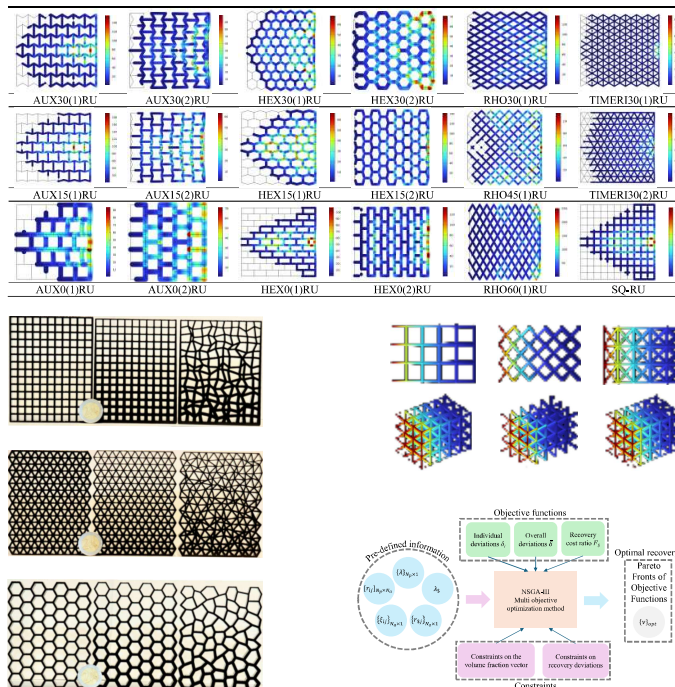




Curriculum 3. Modelling and Simulation

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Mechanics of Lattice Functionally Graded Materials





Doctoral School in Civil, Environmental and Mechanical Engineering
Topic 3. Modelling and Simulation - XXXIII cycle 2021/2024

Doctoral Thesis - December 2025

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Mechanics of Lattice Functionally Graded Materials

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Simulation pictures are created by the author.
The experimental samples have been printed in the Mechano-X Labs



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*To my wife,
who brings spring and calmness to my life.*

Summary

This dissertation investigates the design, modeling, and optimization of architected lattice structures and sustainable composite materials. The work is motivated by the need for lightweight, high-performance materials in modern engineering applications, including aerospace, automotive, civil, and biomedical fields, while also addressing the growing importance of sustainable and recycled material integration.

The research focuses on bridging the gap between classical analytical models, numerical simulations, and data-driven optimization. Classical scaling laws, such as the Gibson–Ashby model, provide a foundation for predicting the mechanical properties of cellular solids, but they are limited in addressing functionally graded structures, structural irregularities, and dynamic behaviors. To overcome these limitations, this dissertation develops extended analytical frameworks, validated through finite element simulations and, where applicable, experimental data.

Key contributions include:

- Development of analytical models for three-dimensional lattices and functionally graded honeycombs, incorporating correction factors to account for grading and randomness.
- Modeling of transient wave propagation in graded lattice structures, including reduced-order, physics-informed approaches that capture dynamic responses efficiently.
- Implementation of a physics-informed, machine learning–driven optimization framework for sustainable composite design, enabling the integration of recycled materials while balancing mechanical performance, economic, and regulatory constraints.
- Methodological exploration of micromechanical methods (MOC, GMC, HFGMC) to establish computational expertise and support data-driven modeling approaches.

By combining analytical, numerical, and data-driven methods, the dissertation provides a comprehensive framework for the design of advanced architected materials and sustainable composites. The work demonstrates both fundamental insights and practical tools for engineering applications, addressing critical gaps in modeling, dynamic analysis, and optimization.

This research lays the foundation for future studies in architected materials, multi-objective design, and sustainable manufacturing, providing guidelines for both theoretical understanding and practical implementation.

Declaration of Author

I, Mohammad Javad Beigrezaee, declare that this thesis titled, "Studying Hierarchical Structures through Functionally Graded Materials" and the work presented in it are my own. I confirm that:

- This work was done wholly or mainly while in candidature for a research degree at this University.
- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- I have acknowledged all main sources of help.

DICAM, University of Trento, Italy, 12th December 2025



Mohammad Javad Beigrezaee

Acknowledgements

I would like to extend my deepest gratitude to those who have supported and contributed to the successful completion of this dissertation. First and foremost, I am profoundly grateful to my advisors, Professor Nicola Maria Pugno and Professor Diego Misseroni, for their invaluable guidance, unwavering support, and insightful feedback throughout my research. Their expertise and encouragement have been instrumental in shaping the direction of this work. I would also like to have a special thank my co-supervisor, Seyed Kamal Jalali, who devoted his time not only to this dissertation but also throughout my Ph.D. program.

I acknowledge the financial support from the European Commission under the H2020 FET Open (“BOHEME”) grant No. 863179 and the Italian Ministry of Education, University and Research (MIUR) under PRIN-20177TTP3S and PRIN-2022ATZCJN-AMPHYBIA, which enabled me to undertake this research and present it effectively.

On a personal note, I would like to express my deepest appreciation to my parents and my sister for their endless patience and encouragement throughout this journey. I am especially grateful to my wife, whose love, support, and understanding have been my constant source of strength.

Thank you all for your contributions and support.

List of publications

- S. K. Jalali, **M. J. Beigrezaee**, D. Misseroni, and N. M. Pugno, “A modified Gibson-Ashby model for functionally graded lattice structures,” *Mechanics of Materials*, vol. 188, p. 104822, Jan. 2024, <https://doi.org/10.1016/j.mechmat.2023.104822>.
- S. K. Jalali, **M. J. Beigrezaee**, N. M. Pugno, “Physically based machine learning for the multi-objective optimal design of partially recycled materials: The case study of rubber resources in the automotive industry”, *Journal of Cleaner Production*, vol. 534, p. 147081, Dec 2025, <https://doi.org/10.1016/j.jclepro.2025.147081>.
- **M. J. Beigrezaee**, S. K. Jalali, D. Misseroni, N. M. Pugno, “A Refined Gibson-Ashby Model for Functionally Graded Honeycombs with Random Irregularities”, *International Journal of Mechanical Sciences*, revised, Under review.
- **M. J. Beigrezaee**, M. Heshmati, S. K. Jalali, N. M. Pugno, “Wave propagation in honeycombs with functionally graded wall thickness and random lattice irregularities”, *International Journal of Mechanical Sciences*, Under review.

List of Conferences

- S. K. Jalali, **M. J. Beigrezaee**, N. Pugno, "Machine Learning-Based Optimization of Recycled Resources Integration in Virgin Materials: A Focus on Automotive Applications", UK Association for Computational Mechanics (UKACM 2025), London, United Kingdom, 23 – 25 April 2025.
- **M. J. Beigrezaee**, S. K. Jalali, D. Misseroni, N. M. Pugno, "Nonlinear Mechanical Simulation of Spider Silk Composites for Enhanced Energy Absorption", 26th International Conference of the Theoretical and Applied Mechanics (ICTAM 2024), Daegu, Korea, 25 – 30 August 2024.
- S. K. Jalali, **M. J. Beigrezaee**, D. Misseroni, N. M. Pugno, "From Silk to Composite: A Nonlinear Micromechanics Approach with Spider Silk Reinforcement and Matrix Variation", 26th International Conference of the Theoretical and Applied Mechanics (ICTAM 2024), Daegu, Korea, 25 – 30 August 2024.
- **M. J. Beigrezaee**, S. K. Jalali, D. Misseroni, N. M. Pugno, "A Gibson-Ashby Model for Graded 2D Cellular Solids", XVII international conference in computational plasticity, fundamentals, and applications (COMPLAS 2023), Barcelona, Spain, 5 – 7 September 2023.

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Introduction

Scientific Trajectory and Motivation

A fundamental challenge addressed early in this research program was the limitation of classical theoretical models, such as the **Gibson-Ashby model**, which assume ideal, periodic structures. Conversely, real-world architected materials frequently exhibit structural complexities, including **Functional Grading variations** and **random irregularities**. The initial phase of this dissertation aimed to systematically refine and extend these classical predictive frameworks to accurately account for the properties of complex, non-ideal lattice architectures. While refining these analytical models provided fundamental insights, the need to perform extensive parametric studies or generate large datasets required for advanced optimization quickly demonstrated the computational expense of traditional methods like FEM. This necessity for efficiency, coupled with the rising importance of data-driven analysis, established a clear path toward incorporating **machine learning** into the research program. To build the necessary computational foundation for this transition, an exploratory study focused on semi-analytical micromechanical methods, specifically the High-Fidelity Generalized Method of Cells (HFGMC). This stage served as a **crucial training ground**, offering a systematic entry point for **learning advanced programming in Python and Julia**. The subcell-based discretization used in HFGMC, which resembles a pixelated grid, naturally aligns with image-processing, preparing the researcher for integrating micromechanical modeling with data-driven workflows. This dissertation thus traces a methodical progression from foundational analytical modeling of non-ideal lattice structures (Chapters 1–3) to the application of physics-informed machine learning and multi-objective optimization for sustainable material management (Chapter 4), with the computational groundwork detailed in the Appendix E.

Core Research Theme I: Static and Dynamic Modeling of Lattices structures (Chapters 1, 2, and 3)

The initial three chapters present a comprehensive investigation into tailoring the mechanical response of cellular structures, moving from foundational static analysis to advanced dynamic mitigation strategies.

The research commenced by extending the classic Gibson-Ashby model for cellular solids to **repetitive graded lattices**. Three well-known porous unit cells, specifically simple cubic, body-centered cubic, and their combination were considered. These graded lattices were geometrically defined by functional variation in the diameters of

the ligaments. A novel analytical framework was developed where the relative density and consequently the relative elastic modulus vary along the graded direction due to gradual changes in the diameters of ligaments. The analytical expressions for the relative elastic modulus were provided by structural analysis of the representative beam framework using the Euler-Bernoulli theory for tapered beams. Closed-form formulas for the effective relative density and the effective relative modulus of fully homogenized FG lattices were subsequently derived. This research showed that the classic Gibson-Ashby model, calibrated only to uniform lattices, is **not accurate** for relating the effective properties of graded lattices. Consequently, a **modified version of the Gibson-Ashby model** was proposed, introducing a correction factor to accurately relate the effective relative modulus to the effective relative density. This framework serves as a practical guideline for designing optimized functionally graded lattice structures, accommodating a wide range of geometric variations.

Building upon the necessity to incorporate non-ideal geometries, the next study refined the Gibson-Ashby equation for predicting the elastic modulus of honeycombs (hexagonal, square, and triangular) exhibiting both functional grading and random irregularities. This directly addressed the critical gap presented by the classical model's reliance on ideal structures. The core contribution involved introducing two correction factors: (κ) to account for FG wall thickness variations, and (η) to capture random irregularities, modifying the equation to: (relative modulus) = ($\kappa\eta C$) (relative density) ^{n} . It was shown that applying the classical Gibson-Ashby equation without modification leads to significant errors. However, by introducing these factors, the classical framework can still provide accurate predictions without altering the power-law exponent (n). These factors were systematically calibrated through a combination of analytical modeling based on Timoshenko beam theory and extensive Finite Element (FE) simulations. Validation against **3D-printed samples** demonstrated the model's capability to predict the reduction in elastic modulus caused by both FG and structural randomness. The proposed framework provides a practical methodology for integrating FG and irregular structures into advanced designs, avoiding high-cost simulations or extensive testing.

The third research area shifted focus to the **dynamic response and impact mitigation** in 2D elastic lattices under transient impact loading. This comprehensive study analyzed 108 lattices, investigating three geometric factors: unit-cell topology, controlled irregularity, and spatial wall-thickness grading (mass shifting). FE simulations confirmed that unit-cell geometry dictates stress wave propagation trajectories. Controlled irregularity was shown to be an effective secondary tuning parameter, particularly when it promotes a switch from stretching- to bending-dominated deformation. A central innovation was the development of an analytical model of graded lattices as a one-dimensional lumped mass-spring system employing the Gibson-Ashby model. This reduced-order, physics-informed model captured the effect of gradually varying wall thicknesses. Results demonstrated that shifting mass toward the impact point reduces input acceleration and transmitted force, significantly improving wave mitigation. This model provides a fast and reliable tool for designing mechanical metamaterials optimized for stress wave attenuation.

Core Research Theme II: Machine Learning and Multi-Objective Optimization for Sustainability (Chapter 4)

Chapter 4 leverages the combined expertise in physics-informed modeling and advanced computation (built upon the foundation established in the Appendix) into a high-impact application addressing sustainable material management challenges. This research introduces a versatile framework that combines **advanced artificial intelligence and multi-objective optimization** with a mathematical model to accelerate the integration of recycled materials into virgin resources. Focusing on recycled rubber from End-of-Life Tires as a case study, the model optimizes the recovery of properties while balancing economic and regulatory constraints. The proposed framework integrates a transparent, semi-analytical micromechanical model with a physics-informed optimization algorithm to manage multiple additive strategies simultaneously. The incorporation of a physics-informed machine learning approach enhances model precision, enabling accurate parameter calibration and effective handling of complex material behaviors. This work establishes a benchmark for sustainable material management, offering a scalable, cost-effective tool to reduce dependency on raw materials and promote recycling efficiency across various industries.

Computational Path: Micromechanical Modeling as a Foundation for Data Science (Appendix)

Following the foundational work on analytical lattice modeling, an exploratory study was conducted on semi-analytical micromechanical methods, including method of cells, generalized method of cells, and the high-fidelity generalized method of cells (HFGMC). This investigation served as a crucial step for developing the necessary computational skills, as the hybrid analytical–computational nature of these methods offered a systematic entry point for **learning advanced programming in Python and Julia**. The structured, subcell-based discretization of these methods resembles a pixelated grid, aligning naturally with image-processing, suggesting their potential for efficient data generation for machine learning applications. The implementation and assessment of HFGMC were primarily motivated by the need to develop the computational expertise required for subsequent chapters, rather than advancing the theoretical formulations of the methods themselves. The detailed documentation of the implementation, performance review, and preliminary results of the HFGMC and related methods is thus included in the Appendix, providing the crucial technical context and preparation for the advanced machine learning investigation presented in Chapter 4.

Dissertation Structure

In summary, this dissertation first establishes modified analytical and theoretical frameworks for accurately predicting the static and dynamic mechanical properties of functionally graded and irregular lattices and honeycombs (Chapters 1–3). It then documents the computational path undertaken to acquire advanced programming skills necessary for data science (Appendix), culminating in the successful integration of physics-based modeling with machine learning and multi-objective optimization to address critical challenges in sustainable material engineering (Chapter 4).

- **Chapter 1:** Static Properties of Functionally Graded Cubic Lattices.
- **Chapter 2:** Static Properties of Functionally Graded and Irregular Honeycombs.
- **Chapter 3:** Dynamic Response and Impact Mitigation in 2D Lattices.
- **Chapter 4:** Machine Learning and Multi-Objective Optimization for Sustainable Material Management.
- **Appendix:** Computational Implementation and Assessment of Micromechanical Methods (MOC, GMC, and HFGMC).

Part I

Lattice structures

CHAPTER 1

A Modified Gibson-Ashby Model for Functionally Graded Lattice Structures

Authors: S. K. Jalali, M. J. Beigrezaee, D. Misseroni, N. M. Pugno

Journal: Mechanics of Materials

Year:2024 | **Vol:**188 | **Page:** 104822

Abstract: The current paper extends the classic Gibson-Ashby model of cellular solids for repetitive graded lattices. Three well-known porous unit cells, i.e., simple cubic (SC), body-centered cubic (BCC), and their combination (BCC⁺), are considered and the corresponding graded lattices are geometrically defined by functional variation in the diameters of the ligaments based on a power law. The analytical expressions for the relative elastic modulus of the cells, which vary along the graded direction, are provided by structural analysis of the representative beam framework containing tapered beams using the Euler-Bernoulli theory. After that, continuous approximation functions for variation of the relative density and the relative elastic modulus are presented by curve fitting over the analytical expressions along the graded direction. Then, the graded lattices are considered to be fully homogenized and as a homogeneous media, the exact expressions for the effective relative density and the effective relative modulus are presented. The modified version of the Gibson-Ashby model is proposed to relate the effective relative modulus to the effective relative density by introducing a correction factor to the classic model. It is shown that the classic Gibson-Ashby model with the coefficients fitted on uniform lattices, is not accurate for relating the effective properties of the graded lattices. The proposed model, presented as an analytical expression with fitting parameters and a correction factor, serves as a useful guideline for designing optimized functionally graded lattice structures, accommodating a wide range of geometric variations.

Highlights:

- The geometry of repetitive graded lattices is parameterized.
- Exact expressions for relative density and modulus are provided.
- The classic Gibson-Ashby model is modified for graded lattices.
- The modified model is validated via simulations.

keywords: Functionally Graded, Gibson-Ashby Model, Repetitive Lattice structures, Porosity, Additive manufacturing.

1.1 Introduction

Thanks to the recent technological advances in manufacturing methods, material scientists and designers have encountered a wide variety of novel material selections in conjunction with the possibility of producing complex geometries to accurately match the desired properties according to demanded applications. Among them, the idea of Functionally Graded (FG) change in material properties is one of the great choices due to its exceptional potential in a wide range of industrial applications such as automotive [1, 2], aerospace [3, 4], biomedical [5, 6], etc. [7–9]. In addition to the conventional composite FG materials where the functional change is only imposed by graded variation in the volume fraction of components, new additive manufacturing methods [10] suggest fabrication of advanced cellular solids [11] as lattice structures with complex graded structural architectures by functional variation in the geometrical parameters of the cells. Not only the distribution of the type and the size of unit cells within the lattice structure can be varied in different directions but also each of the unit cells can have graded changes in the thickness of ligaments that affect the whole structural performance. Therefore, this class of porous materials possesses a remarkable perspective to replace conventional materials in many industrial applications, and hence the investigation of their properties is of particular importance [12]. They are also of interest in the field of metamaterial science [13–15].

From the analytical point of view, the mechanical properties of a porous cellular solid can be evaluated by common analytical structural theories derived from various geometric microstructure models [16–19]. One of the most applied formulas, which is widely implemented for the open- and closed-cell foams and structures, is the power law [20], introduced by Gibson and Ashby [11, 17]. This model relates the fundamental mechanical properties of lattice structure to its density, defining the relative properties of the lattice as the ratio of its properties to the bulk counterpart. The Gibson-Ashby model has two constants, one of which is the power of the relative density (usually denoted by n) and the second one is the multiplier (usually denoted by C). For many cases, these two constants should be fitted with the existing data for accurate results while for simplicity, they are set for some general lattice structure as a unique value. For instance, for an open-cell foam, n is usually set to 2 and C is equal to 1 for evaluating the stiffness modulus. Although some literature [21, 22] reported that these values for the Gibson-Ashby theory can predict the mechanical behavior with good accuracy, some other researchers [23–25] showed that these constants should be modified according to the material and the fabrication procedure from which the cellular solid is made [26].

The other reason why the Gibson-Ashby model should be fitted case by case is that different architectures for each of the unit cells of lattice structures significantly affect the mechanical response under loading. Accordingly, the mechanical properties of lattice structures have been analytically investigated by recent studies due to the advances in the additive manufacturing method, which allows the production of different types of complex unit cells. [27]. Hedayati et al. [28] derived an analytical solution

for evaluating the mechanical properties of the porous structure made of truncated cube unit cells. Besides, they developed a finite element (FE) model and compared the results with the analytical ones. Elastic modulus and Poisson's ratio of a lattice structure with the body-centered cuboid unit cell have been analytically evaluated by Ptochos and Labeas [29]. While the well-known unit cell called body-centered cubic (BCC) has equal dimensions in all directions, the body-centered cuboid, on the other hand, has unequal dimensions in three directions. Both Timoshenko and Euler-Bernoulli's beam theories were applied to analyze the structure under complex loading conditions. Finally, they claimed that their approach is a cost-efficient method for evaluating the mechanical behavior of the lattice structure made of BCC or body-centered cuboid. Classical beam theory had been applied [30] for evaluating the initial specific stiffness of a BCC lattice structure. The results showed that the aspect ratio of the ligaments directly affects the accuracy of the results.

All the mentioned studies were on finding the properties of uniform lattice structures with constant geometrical and material properties of the unit cell, benefiting the Gibson-Ashby model for prediction. In parallel, some other researchers in the field of structural analysis tried to extend these formulations for uniform lattices to functionally graded porous (FGP) structural members, i.e., beams, plates, panels, shells, etc., where the porosity varies continuously within the member mostly in the direction of thickness. For this purpose, they assumed the same Gibson-Ashby model with the same parameters, mostly $n = 2$ and $C = 1$ fitted for uniform open-cell lattices, in order to define the function of variation in mechanical properties for FGP structural members and found their mechanical response under different load conditions [31, 32]. By use of the pseudo-spectral method, Jalali and Heshmati [33] numerically computed the governing equations for free vibration of the FGP circular plates where the porosity gradually changes along the radial direction and the effect of different porosity distributions alongside different boundary conditions were presented. In another study [34], they investigated the effect of tapering on the FGP circular and annular plates having variable properties along the radial direction, and the potential of thickness variation profile for optimizing the frequency response was examined. Jalali et al. [35], probed the possibility of extending the closed-form solutions of homogeneous plates under different loading conditions to the FGP ones. Many case studies were performed and they claimed that it was not necessary to resolve the governing equation of the plate theories for the plates with FGP along the thickness since the available exact solutions in the literature on homogeneous plates could be used by substituting the corresponding out-of-plane and in-plane rigidity and moments of inertia of FGP plate. Therefore, they presented the exact expression of these rigidities and moments of inertia for 12 different porosity distributions by integrating them across the thickness. In a recent study [31], a misunderstanding was reported regarding the relationship between the mechanical properties of FGP structures and density. The study established a local (point-by-point) version of the Gibson-Ashby model. They showed that this misunderstanding which is observed in a large number of publications in the literature led to an undeniable error in predicting both the statics and dynamics mechanical response of the FGP structure.

According to Bai et al. [36], FGP materials can be divided into four categories including changing the material properties, changing the unit cell type, scaling the unit cell, and changing the diameter of the unit cell ligaments which the latest one has the most structural integrity compared to the other methods. The results showed that their new configuration, which was based on BCC unit cells, had a great capability of absorbing energy under large strain and efficient support under small strain. They also claimed that the Gibson-Ashby theory could accurately predict the mechanical properties of their lattice configuration. In continuing this work, Rodrigo et al. [37] studied the deformation pattern of an FG lattice structure based on BCC unit cells and compared it with the uniform one. Maskery et al. [38] considered the standard BCC unit cell and its reinforced version by adding struts in the direction of applied load (named BCC_z) in order to compare the collapse deformation process from the video recording with the properties of the stress-strain diagram. Choy et al. [39] experimentally studied the energy absorption of FG cubic and honeycomb lattice structures with graded changes in the diameter of ligaments fabricated by selective laser melting (SLM), with Ti-6Al-4V as the building material and showed that the energy absorption capability is significantly affected by the direction of loading. In other two related studies, Al-Saedi et al. [40] and Al-Saedi and Masood [41] described energy absorption capacity and mechanical properties of uniform and FG lattice structure using the combination of BCC and face-centered cubic unit cell, called F2BCC, and the general conclusion is similar to those reported in [38] and [39] saying that the uniform lattice structure had a shear failure mode of 45° at its peak of compression stress. However, FG lattice structures obviously collapsed layer by layer consecutively from the lowest to the highest density layer. In addition, the FG lattice structure with F2BCC unit cells showed higher energy absorption despite the earlier beginning of densification strain compared to the uniform one. They also announced that the cumulative energy absorption per unit volume as a function of strain was increased exponentially for FG lattice structure, while it was bilinear for uniform one. Mahbod and Asgari [42] introduced a new configuration for the unit cell of FG structures by a step-wise change in the diameters of ligaments (layer by layer of cells along the graded direction) and characterized the elastic and plastic properties via an analytical model which was previously provided in [28, 43]. While a good correlation between analytical, numerical, and experimental data was obtained, they claimed that the new unit cell could be compatible with various applications because of the versatile design methodology for manufacturing the desired material properties. In one of the most recent studies, a new unit cell, containing 16 connection nodes and 32 inclined struts, was introduced by Gharehbaghi et al. [44] and the elasticity modulus in two directions along with Poisson's ratio were assessed via the equations of Euler-Bernoulli beam theory and the effect of step changes in the diameter of struts as an FG graded lattice is investigated. They also analyzed the layer-wised FG structure with three overall porosity and the numerical and experimental results revealed a good correlation with the analytical ones.

To the best knowledge of the authors, there is no exact analytical solution for evaluating the relative density and the relative stiffness modulus of FG lattice structures.

Therefore, the current paper aims to parameterize the variation in the architecture of these nonuniform lattices with a variable diameter of ligaments for different types of common unit cells in order to find the analytical expression for evaluating the relative density and stiffness modulus. Among the huge library of unit cells with exceptional mechanical properties, [45–47], three well-known unit cells, i.e., simple cube, body-centered cubic, and their combination are selected. Next, from a fully homogenized point of view, the closed-form formulas for the effective density and effective modulus of FG lattices are derived. Besides, approximation functions for the estimation of the relative density and the relative elastic modulus along the graded direction are presented by the use of curve fitting over analytical solutions. Finally, a modified Gibson-Ashby model with a correction factor is introduced which can relate accurately the effective relative stiffness modulus to the effective relative density. The presented calibrated correction factor covers a wide range of variations in the diameter of the ligament for three types of considered unit cells.

1.2 Methodology

1.2.1 The geometric definition of graded lattices

Consider a cubic unit cell of a length side l and a main diagonal $\sqrt{3}l$ which can construct three well-known lattices i.e., simple cubic (SC) where only the sides of the cube are kept, the body-centered cubic (BCC) where only the main diagonals are kept, and their combination (BCC⁺). One should note that in a 3D repetition, every side is shared between four neighboring cells, while the diagonals belong exclusively to the cell. A lattice structure is built up by placing the ligaments of nominal diameter d on the sides and/or the diagonals. It is useful to define the dimensionless ratio of a ligament, $R = d/l$, for the purpose of generality.

A graded lattice structure can be achieved in three ways: First, a gradual change in the properties of the bulk material having a uniform lattice geometry, second, a gradual change in the lattice constant fixing the bulk material and the diameter of ligaments, and third, a gradual change in the diameter of ligaments keeping constant the bulk material and the lattice constant. Here, the last one is selected because the first one faces the difficulties of multi-material fabrication, and the second, although is identical to the idea of gradual change in the pore size for an irregular 3D foam, presents difficulties when it is applied to a regular lattice. Figure 1.1 illustrates the schematic of the functionally graded lattice under study. It is assumed that the dimensionless diameter of ligaments, R , varies along x axis, through N cells with the total length of $L = Nl$ from R_0 at $x = 0$ to R_N at $x = L$. Because of the discontinuous nature of lattice, the variation function should be defined in a clear way for all the ligaments which are categorized into three groups: those lying on the sides of cubes on the $y - z$ planes, those on the sides of the cubes parallel to the gradual direction, i.e., x , and those placed on the diagonals. The definition of the graded lattice starts with

the first category, where it is assumed that the dimensionless diameter of ligaments laid on $y - z$ planes varies according to a power law as follows:

$$R_{yz}^{(j)} = R_0 + \Delta R \left(\frac{j}{N} \right)^m \quad (1.1)$$

where $\Delta R = R_N - R_0$ and $j = 1, 2, \dots, N$. Then, the ligaments parallel to x axis as well as the diagonal ones are divided by N interval placed among $N + 1$ groups of ligaments on $y - z$ planes. The ligaments parallel to the x axis are assumed to have a tapering variation forming conical frustums. For k th cell, $k = 1, 2, \dots, N$, the ending diameters of the conical frustum ligaments are equal to $R_{yz}^{(k-1)}$ and $R_{yz}^{(k)}$ correspond to the $(k - 1)$ th and k th $y - z$ planes defined by Equation (1.1):

$$R_{yz}^{(k-1)} = R_0 + \Delta R \left(\frac{k-1}{N} \right)^m \quad (1.2a)$$

$$R_{yz}^{(k)} = R_0 + \Delta R \left(\frac{k}{N} \right)^m \quad (1.2b)$$

The diameter of diagonal ligaments in k th cell is assumed to be constant and equals to the average diameter of the $(k - 1)$ th and k th $y - z$ planes as:

$$R_{ave}^{(k)} = \frac{R_{yz}^{(k-1)} + R_{yz}^{(k)}}{2} = R_0 + \frac{\Delta R}{2N^m} ((k-1)^m + k^m) \quad (1.3)$$

It results in a step-wise change in the diameter of diagonal ligaments in N steps. Figure 1.2 presents a sample of the three graded lattice structures with a linear power law variation, $m = 1$, from a thin to a thick dimensionless diameter, $R_0 = 0.05$ to $R_N = 0.5$, with a resolution of $N = 20$. As seen, for a linear variation swapping R_0 and R_N does not modify the geometry and the graded lattice only rotates 180° . However, this is not the case for $m \neq 1$. The effect of swapping $R_0 = 0.05$ and $R_N = 0.25$ on the geometry of a sample BCC⁺ graded lattice is demonstrated in Figure 1.3 for $m = 3$ resulting in a considerable difference in the variation of density and mechanical properties along the graded axis, x .

1.2.2 The relative density of graded lattices

The relative density of a cell is defined as the volume ratio of the lattice, ρ , to the bulk, ρ_0 . It can be approximated based on the assumption that the volume of the lattice simply equals the sum of the volume of the ligaments ignoring the overlaps in the joints [11], however, it overestimates the relative density, especially for higher values of R due to high overlapping volume. Hence, the correction factor, $\gamma < 1$ is introduced to fit the approximation to the exact values. For the special case of uniform unit cells with ligaments of identical diameter, it results in the following relative densities:

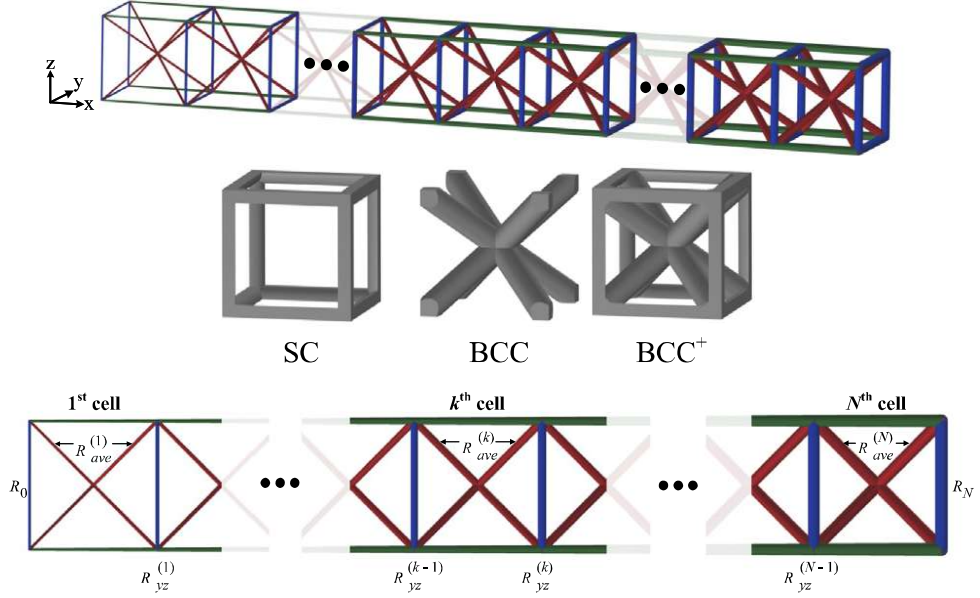


Figure 1.1. The schematic of the graded lattice structure and the three possible unit cells.

$$\left(\frac{\rho}{\rho_0}\right)_{SC}^{(0)} = \left(\frac{V_{cell}}{V_0}\right)_{SC}^{(0)} = \gamma_{SC}(3\pi/4)R^2 \quad (1.4a)$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC}^{(0)} = \left(\frac{V_{cell}}{V_0}\right)_{BCC}^{(0)} = \gamma_{BCC}\pi\sqrt{3}R^2 \quad (1.4b)$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC^+}^{(0)} = \left(\frac{V_{cell}}{V_0}\right)_{BCC^+}^{(0)} = \gamma_{BCC^+}\pi(3/4 + \sqrt{3})R^2 \quad (1.4c)$$

where V_{cell} is the total volume of ligaments without overlaps and $V_0 = l^3$ is the volume of the bulk unit cell (see A.1). For the SC lattice, a closed-form expression for evaluating the overlaps in an orthogonal junction of cylinders and consequently the exact value of γ_{SC} is available, however, for the BCC and BCC⁺ lattices the least square approach is used to find the best fitted γ to the exact relative densities obtained from the exact CAD models:

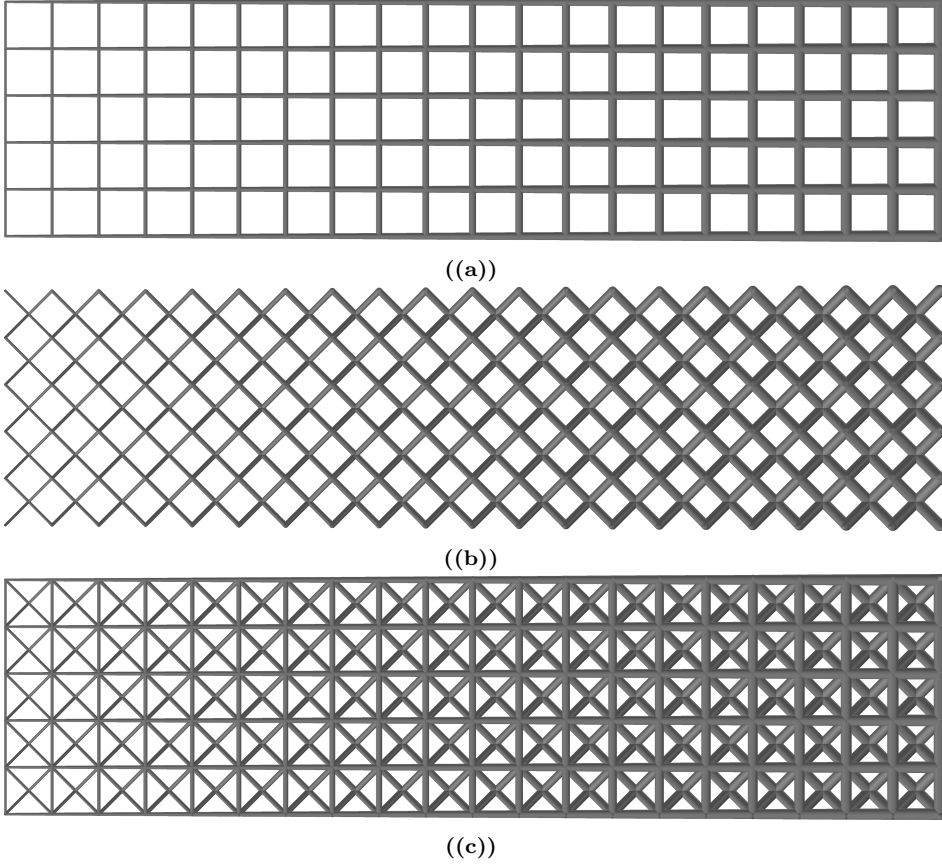


Figure 1.2. Sample graded lattice structures with a linear ($m = 1$) variation of dimensionless diameter of ligaments R , from $R_0 = 0.05$ to $R_N = 0.25$ for a) SC, b) BCC and c) BCC⁺ unit cells.

$$\left(\frac{\rho}{\rho_0}\right)_{exact} = \gamma \left(\frac{\rho}{\rho_0}\right)_{approx} \quad (1.5a)$$

$$\gamma_{SC} = 1 - \frac{4\sqrt{2}}{3\pi}R \approx 1 - 0.600R \quad (1.5b)$$

$$\gamma_{BCC} = 1 - 0.900R \quad (1.5c)$$

$$\gamma_{BCC^+} = 1 - 1.1088R \quad (1.5d)$$

In Figure 1.4 the approximation is compared to the exact relative density across the dimensionless diameter range of $0.05 < R < 0.5$ which reveals the undeniable error for $R > 0.2$

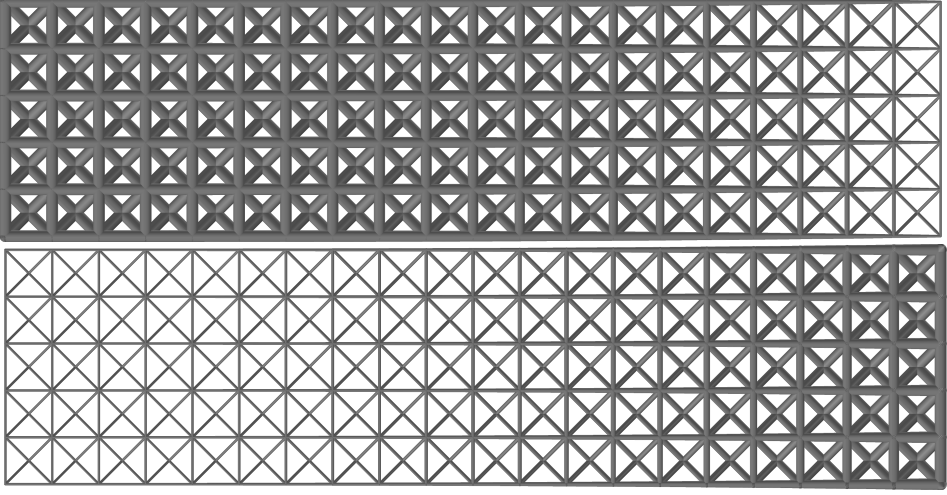


Figure 1.3. The influence of swapping the values of $R_0 = 0.05$ and $R_N = 0.25$ for a graded BCC⁺ lattice with $m = 3$.

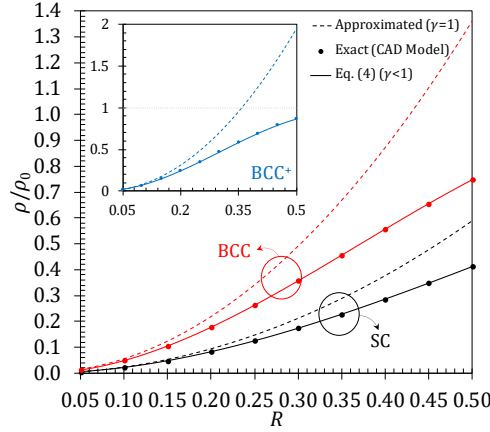


Figure 1.4. Comparison of the modified relative density (Equation (1.4) with $\gamma < 1$ obtained from the curve fitting to the CAD model) with the approximate one ($\gamma = 1$) for SC, BCC, and BCC⁺ uniform lattices.

In a graded lattice, R is not constant and varies from R_0 to R_N via Equation (1.1) with the power m . One can obtain the relative density of k th cell as a function of R_0 and ΔR as follows (for more details on the calculations see A.1):

$$\left(\frac{\rho}{\rho_0}\right)_{SC}^{(k)} = \gamma_{SC}^{(k)} \left[a_1^{(k)} R_0^2 + a_2^{(k)} (\Delta R)(R_0) + a_3^{(k)} \Delta R^2 \right] \quad (1.6a)$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC}^{(k)} = \gamma_{BCC}^{(k)} \left[a_4^{(k)} R_0^2 + a_5^{(k)} (\Delta R)(R_0) + a_6^{(k)} \Delta R^2 \right] \quad (1.6b)$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC^+}^{(k)} = \gamma_{BCC^+}^{(k)} \left[a_7^{(k)} R_0^2 + a_8^{(k)} (\Delta R)(R_0) + a_9^{(k)} \Delta R^2 \right] \quad (1.6c)$$

where the coefficients $a_i^{(k)}$ are functions of k , the number of lattices along the graded direction, N , and the power m presented in A.1. To diminish the error caused by overlaps in the joints of graded lattices, the correction factor obtained for uniform unit cells in Equation (1.5) is extended to the k th unit cell, $\gamma^{(k)}$, by substituting R with the average dimensionless diameter $R_{ave}^{(k)}$ defined in Equation (1.3). Note that Equation (1.6) is simplified to the special case of uniform lattice presented in Equation (1.4) and Equation (1.5) by setting either $\Delta R = 0$ or $m = 0$.

1.2.3 The analytical solution for relative elastic modulus of k th cell in the graded lattices

In this subsection, the analytical expression for the relative elastic modulus i.e., the stiffness ratio of the lattice, E , to the bulk, E_0 , is presented based on the Euler-Bernoulli beam theory. For the graded lattices, the relative elastic modulus is not constant along the graded direction, x , due to the variation of dimensionless diameters of ligaments, R . Reminding Equation (1.1) and Equation (1.3) which define the dimensionless diameter of the ligaments constructing the k th cell of the graded lattice, and a tapering variation in the diameter of the ligaments parallel to x , the relative elastic modulus for the k th unit cell is obtained by (see A.2 for the details of calculations):

$$\left(\frac{E}{E_0}\right)_{SC}^{(k)} = \frac{\pi}{4} R_{yz}^{(k-1)} R_{yz}^{(k)} \quad (1.7a)$$

$$\left(\frac{E}{E_0}\right)_{BCC}^{(k)} = \pi \sqrt{3} \left(\frac{(R_{ave}^{(k)})^4}{2 + (R_{ave}^{(k)})^2} \right) \quad (1.7b)$$

$$\left(\frac{E}{E_0}\right)_{BCC^+}^{(k)} = \frac{b_1^{(k)} b_2^{(k)}}{b_1^{(k)} + b_2^{(k)}} \quad (1.7c)$$

where the coefficients $b_1^{(k)}$ and $b_2^{(k)}$ are presented in A.2. For the special case of uniform lattices with all the ligaments with identical dimensionless diameter, R , the relative stiffnesses of SC, BCC, and BCC⁺ are:

$$\left(\frac{E}{E_0}\right)_{SC}^{(0)} = \frac{\pi}{4} R^2 \quad (1.8a)$$

$$\left(\frac{E}{E_0}\right)_{BCC}^{(0)} = \pi\sqrt{3} \left(\frac{R^4}{2 + R^2}\right) \quad (1.8b)$$

$$\left(\frac{E}{E_0}\right)_{BCC^+}^{(0)} = \frac{\pi}{4} \left(\left(1 + \frac{4\sqrt{3}}{9}\right) R^2 + \frac{8\sqrt{3}}{9} R^4 \right) \quad (1.8c)$$

1.2.4 The equivalent function for density and elastic modulus of functionally graded lattices

A lattice structure is naturally a discontinuous non-homogeneous media and the exact value of density and elastic modulus at a given point (x, y, z) within the media is either the bulk density or zero according to whether the point is located on the ligaments or not (Figure 1.5).

As the first level of homogenization, one can assume that the lattice structure within a unit cell space is a continuous homogeneous media with an equivalent density/modulus equal to the relative density/modulus of the cell, discussed respectively in Section 1.2.2 and Section 1.2.3. However, as presented in Equation (1.6) and Equation (1.7), the relative density, as well as the relative elastic modulus of the unit cells of a graded lattice structure, are not constant resulting in a step-wise variation along the direction of graduation which is x axis here (see Figure 1.5). This subsection aims to suggest an approximation for the variation of relative density and relative elastic modulus as functions of x , i.e., $\rho(x)/\rho_0$ and $E(x)/E_0$. Since the variation of the diameters of ligaments with respect to x obeys a power law (Equation (1.1)), the same form of approximation function is chosen:

$$\left(\frac{\rho(x)}{\rho_0}, \frac{E(x)}{E_0}\right) \approx (p_1, q_1)x^{(\alpha, \beta)m} + (p_2, q_2) \quad (1.9a)$$

$$(p_1, q_1) = \frac{\left(\frac{\rho}{\rho_0}, \frac{E}{E_0}\right)^{(N)} - \left(\frac{\rho}{\rho_0}, \frac{E}{E_0}\right)^{(1)}}{l^{(\alpha, \beta)m}((N - 0.5)^{(\alpha, \beta)m} - 0.5^{(\alpha, \beta)m})} \quad (1.9b)$$

$$(p_2, q_2) = \left(\frac{\rho}{\rho_0}, \frac{E}{E_0}\right)^{(1)} - (0.5l)^{(\alpha, \beta)m}(p_1, q_1) \quad (1.9c)$$

where $(\ , \)$ represents *or* which means p_1 , p_2 , and α belongs to the density, while q_1 , q_2 , and β are related to the elastic modulus. In Equation (1.9), the relative

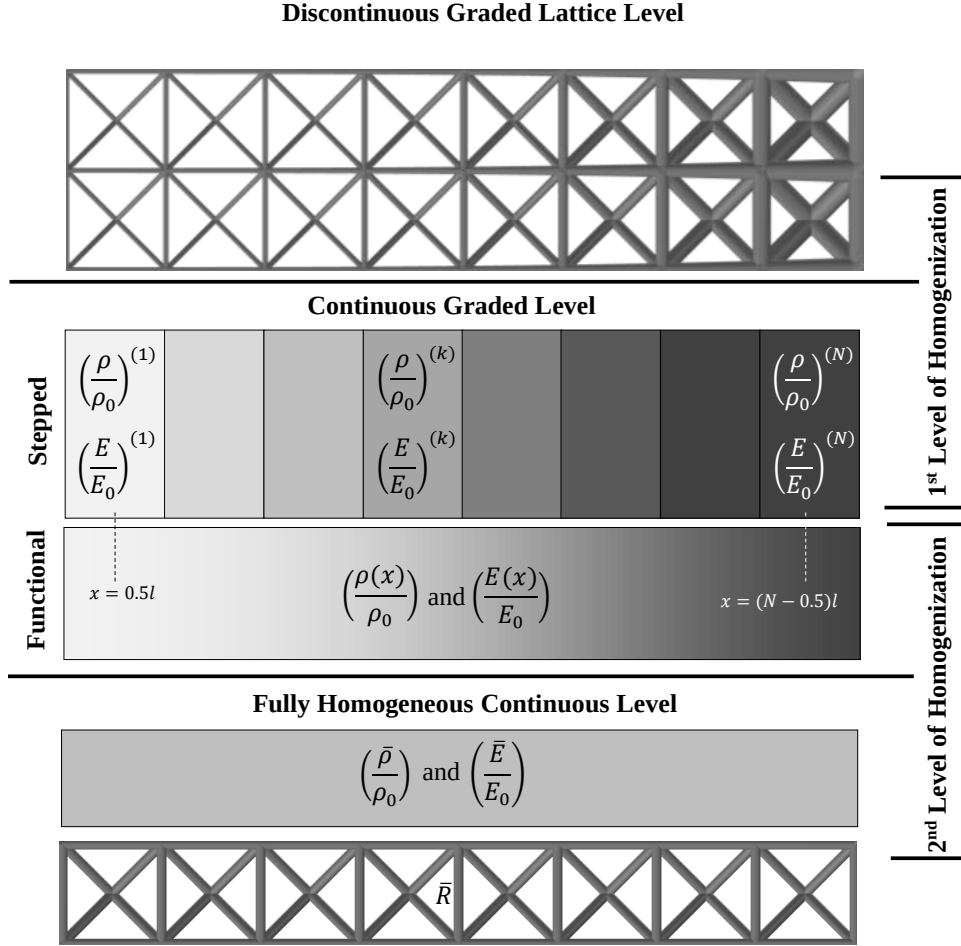


Figure 1.5. The first and the second levels of homogenization of the graded lattices.

density/modulus of the first ($k = 1$) and the last ($k = N$) unit cells obtained from Equation (1.6) and Equation (1.7) has assigned to the coordinate of their center, i.e., $x = 0.5l$, and $x = (N - 0.5)l$, see Figure 1.5. The power m is modified by α and β fitting parameters as the variation of relative density/modulus with respect to x has not necessarily an identical power to the variation of the dimensionless diameter due to the discontinuous nature of the lattice. The calibrated values of α and β corresponding to different values of R_0 and R_N for SC, BCC, and BCC⁺ lattices are presented in both graphical forms and fitting equations in A.3. The second possible level of homogenization for graded lattices is performed by introducing the effective

density, $\bar{\rho}$, and the effective elastic modulus, $\bar{E}$, as shown in Figure 1.5. $\bar{\rho}$ is the density of a fully homogenized material whose mass is equal to the mass of a graded lattice with N cells along the graded axis, while both of them have occupied the same volume of Nl^3 . As the lattice structure is regular and all the cells have the same volume, l^3 , the effective density, $\bar{\rho}$, is simply the average of the density of cells:

$$\frac{\bar{\rho}}{\rho_0} = \frac{1}{N} \sum_{k=1}^N \left(\frac{\rho}{\rho_0} \right)^{(k)} \quad (1.10)$$

which is divided by the bulk density, ρ_0 , to be compatible with the representation in Equation (1.6) for SC, BCC, and BCC⁺ lattices. If the approximated continuous function for the density of graded lattice, $\rho(x)$ is used, Equation (1.10) turns to an integration form:

$$\frac{\bar{\rho}}{\rho_0} \approx \frac{\int_0^{Nl} \left(\frac{\rho(x)}{\rho_0} \right) dx}{Nl} \quad (1.11)$$

Substituting Equation (1.9) into Equation (1.11) yields:

$$\frac{\bar{\rho}}{\rho_0} \approx \frac{p_1(Nl)^{(\alpha m)}}{\alpha m + 1} + p_2 \quad (1.12)$$

After the first level of homogenization, the graded lattice converts to N unit cells with the elastic modulus of $E^{(k)}$, $k = 1, \dots, N$, connected in series. Under an applied load in the grading direction, P , the total elongation of the graded structure is:

$$\delta_{graded} = \frac{Pl}{l^2} \sum_{k=1}^N \frac{1}{E^{(k)}} \quad (1.13)$$

The elongation of a fully homogenized material with the same cross-section area of l^2 and length Nl is:

$$\bar{\delta} = \frac{PNl}{l^2 \bar{E}} \quad (1.14)$$

One can find the effective modulus of the graded lattice by assuming $\delta_{graded} = \bar{\delta}$ and solving for $\bar{E}$:

$$\frac{\bar{E}}{E_0} = \frac{N}{\sum_{k=1}^N \frac{1}{(E/E_0)^{(k)}}} \quad (1.15)$$

which is divided by the bulk elastic modulus, E_0 , to be compatible with the representation in Equation (1.7) for SC, BCC, and BCC⁺ lattices. The integration form of Equation (1.15) can be obtained by using the continuous approximation of elastic modulus from Equation (1.9) for evaluating the elongation of graded lattice, δ_{graded} , which results in:

$$\frac{\bar{E}}{E_0} \approx \frac{Nl}{\int_0^{Nl} \frac{1}{(E(x)/E_0)} dx} \quad (1.16)$$

Note that substituting Equation (1.9) into Equation (1.16) demands a numerical integration as the exact solution is not available.

It is useful to introduce a uniform lattice with a constant dimensionless diameter, $\bar{R}_\rho$, which results in the same effective relative density (same mass) by equating Equation (1.12) to Equation (1.4) considering the correction factor defined in Equation (1.5) and solving for R :

$$\left(\frac{\bar{\rho}}{\rho_0} \right) = \left(\frac{\rho}{\rho_0} \right)^{(0)} \quad (1.17)$$

Similarly, the dimensionless diameter of a uniform lattice with the same effective relative modulus, $\bar{R}_E$, can be obtained by solving the following equation for R :

$$\left(\frac{\bar{E}}{E_0} \right) = \left(\frac{E}{E_0} \right)^{(0)} \quad (1.18)$$

The effective density and effective elastic modulus for SC, BCC, and BCC⁺ lattices and for three different power, $m = 1, 2$, and 3 are graphically presented in A.4 using the exact expressions in Equation (1.10) and Equation (1.15).

1.2.5 The modified Gibson-Ashby model for graded lattices

According to the classical Gibson-Ashby model for a uniform cellular solid, the relative elastic modulus is related to the relative density as:

$$\left(\frac{E}{E_0} \right)^{(0)} = C^{(0)} \left(\left(\frac{\rho}{\rho_0} \right)^{(0)} \right)^{n^{(0)}} \quad (1.19)$$

where $C^{(0)}$ and $n^{(0)}$ are the fitting parameters. The modified Gibson-Ashby model is established based on the assumption that the original expression in Equation (1.19) is also valid for the relationship between the effective relative modulus and the effective relative density given in Equation (1.10) and Equation (1.15), respectively:

$$\left(\frac{\bar{E}}{E_0} \right) = \kappa C^{(0)} \left(\frac{\bar{\rho}}{\rho_0} \right)^{n^{(0)}} \quad (1.20)$$

in which κ is the correction factor that modifies the original relationship of uniform lattices for the graded ones. It is reasonable to assume that κ is a function f of the degree of gradual changes in the lattice geometry, which is controlled by the ratio (R_N/R_0) and the power m :

$$\kappa = f((R_N/R_0), m) \quad (1.21)$$

The calibrated values of κ are presented in A.5. The special case is when $(R_N/R_0) = 1$ or $m = 0$ resulting in a uniform lattice with $\kappa = 1$.

In addition to the fully homogenized effective properties, it is of interest to look at the graded lattice from a local (cell by cell) point of view, where the relative density and the relative elastic modulus vary along the graded direction, x , according to Equation (1.9). One may suggest relating them to implementing the local version of the classical Gibson-Ashby model:

$$\left(\frac{E(x)}{E_0} \right) = C^{(0)} \left(\frac{\rho(x)}{\rho_0} \right)^{n^{(0)}} \quad (1.22)$$

However, another choice is to update the local version with the modified model by introducing the correction factor κ in Equation (1.22):

$$\left(\frac{E(x)}{E_0} \right) = \kappa C^{(0)} \left(\frac{\rho(x)}{\rho_0} \right)^{n^{(0)}} \quad (1.23)$$

The comparison between the accuracy of Equation (1.22) and Equation (1.23) for different combinations of the dimensionless diameters R_0 , R_N , the power m , and for SC, BCC, and BCC⁺ lattices is presented and discussed in Section 1.3.

1.2.6 The finite element method (FEM) validation study

Here, a numerical model based on FEM employing the commercial software, COMSOL Multiphysics[®], is presented which is used to check the correctness and the validity of the developed analytical formulation. Two different sets of FEM simulations are performed: the unit cell simulations (FE-UC) and the lattice simulations (FE-Lattice). The FE-UC model considers the smallest representative structural element of the lattices, exactly the same as the assumption in A.2, by modeling the beam frames and the boundary conditions defined in Figure A.2, Figure A.3, and Figure A.4 for the SC, BCC, and BCC⁺ lattices, respectively. Due to its unit cell-based approach, the FE-UC simulations are only applicable for checking the prediction of uniform lattices since the graded lattice needs a row of cells to define a graded change in the diameters of ligaments. To see the effect of shear deformation both Euler-Bernoulli and Timoshenko beam theories are applied to the FE-UC model. On the other hand, for the FE-Lattice simulations, a sample representative lattice consisting of 45 unit cells is modeled where $N = 5$ is the number of unit cells along the graded direction (and also load direction) and $3 \times 3 = 9$ unit cells are laid on the cross-sections. Figure 1.6 presents the schematic of the representative lattice for the SC lattice.

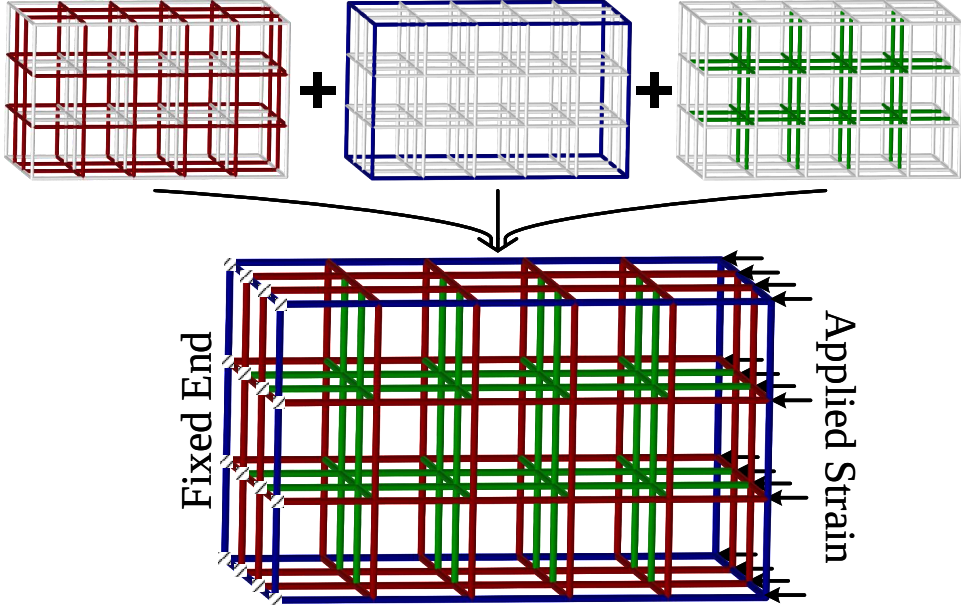


Figure 1.6. The representative lattice of the FE-Lattice simulations.

It is assumed that the representative lattice is a section of a whole larger lattice and therefore, the ligaments on the outer skin are shared and do not completely belong to the representative lattice. Hence, the cross-section area of the ligaments on the lateral surfaces, the red ones, is divided by two (the diameter is divided by $\sqrt{2}$), while the cross-section area of the ligaments on the edges, the blue ones, is divided by four (the diameter is divided by 2). The cross-section of the ligaments within the representative lattice, green ones, is not modified. Note that for the BCC lattice, all the ligaments are within the lattice and are green. The boundary condition is applied as follows: For the 16 nodes on the right end of the lattice in Figure 1.6, all the rotations are fixed and an arbitrary displacement along the graded direction, x , is applied. For the 16 nodes on the left end, all the rotations are fixed and the displacement along the x axis is fixed. Finally, for the rest of the boundary nodes on the lateral surfaces, the rotations are fixed. Since the developed analytical formulation is based on the Euler-Bernoulli beam theory, the same theory is employed for the FE-Lattice simulations. In both FE-UC and FE-Lattice simulations, every ligament with a circular cross-section is discretized by 10 quadratic meshes to guarantee independence from the mesh. Figure 1.7 shows a sample of displacement field contours for the lattices with $R_N/R_0 = 3$ and $m = 1$.

The equivalent stress is calculated by dividing the resultant reaction force along the x axis on the fixed nodes on the left to the cross-section area of the model perpendicular to the x axis, and the equivalent strain is obtained by dividing the

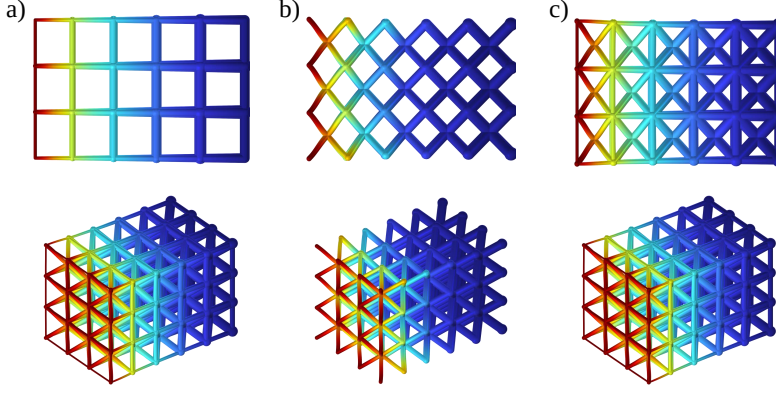


Figure 1.7. Sample displacement fields along the applied strain direction from FEM-Lattice simulation for a) SC, b) BCC, and c) BCC⁺ lattices with $R_N/R_0 = 3$ and $m = 1$. The presented color maps are relative in order to show the distribution of the displacement field within the structure. Red represents the highest and blue is the lowest displacement.

applied displacement by the length of the model along the x axis. Then, the effective modulus is calculated by dividing the equivalent stress by the equivalent strain.

1.3 Results and discussion

1.3.1 Analytical and numerical results

In this section, the validity of the proposed analytical model for graded lattices is examined and the question "How accurate is it to apply the classical Gibson-Ashby model with the coefficients obtained from uniform lattices for graded lattices with the same unit cell type?" is answered.

First of all, the accuracy of the approximated continuous functions for variation of the relative density, $\rho(x)/\rho_0$, and relative elastic modulus, $E(x)/E_0$, along the graded direction, x , presented in Equation (1.9), is studied. A high degree of variation of dimensionless diameter is considered by setting $R_0 = 0.05$, and $R_N = 0.25$ which means the diameter of ligaments increases 400% along the graded direction ($R_N/R_0 = 5$). Three different power for the variation function is assumed, $m = 1, 2$, and 3 to test the accuracy of Equation (1.9) covering a broad range of changes in the geometry of the graded structure. Besides, the number of cells along the x axis is $N = 20$ to check the sensibility of approximated functions to the resolution of graded lattice, since the curve fitting parameters, α and β , presented in A.3 are obtained from a high resolution of $N = 100$.

Figure 1.8 compares the continuous function of relative density, $\rho(x)/\rho_0$, with the exact relative densities in Equation (1.6) at the center of cells along x for SC, BCC, and BCC⁺ lattices with the corresponding fitting parameters, $\alpha_{SC} = 1.5$, $\alpha_{BCC} = 1.44$, and $\alpha_{BCC^+} = 1.39$, which can be read from Figure A.6 (A.3) with $R_0 = 0.05$, and $R_N = 0.25$. A good fitting is observed for all the lattices and the powers through

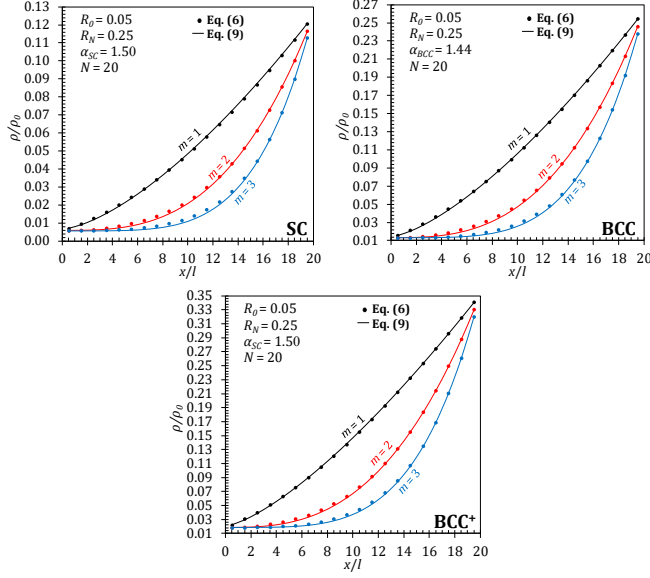


Figure 1.8. The variation of relative density along the graded axis x and the accuracy test of the fitting function presented in Equation (1.9).

the whole length of the graded lattice confirming the accuracy of Equation (1.9) for evaluating the relative density even at a lower resolution, $N = 20$.

The same comparison is performed in Figure 1.9 between the continuous function of relative elastic modulus, $E(x)/E_0$, with the exact relative densities of cells presented in Equation (1.7). The corresponding fitting parameters, $\beta_{SC} = 1.6$, $\beta_{BCC} = 2.94$, and $\beta_{BCC^+} = 1.65$ can be evaluated from Figure A.7 (A.3). Again, a remarkable matching is seen which confirms the accuracy of Equation (1.9) for the relative elastic modulus along the graded direction. Furthermore, the inverses of relative elastic modulus are compared in Figure 1.9 for the three unit cells and one can perceive that $(E(x)/E_0)^{-1}$ does not match accurately the $((E/E_0)^{(k)})^{-1}$ especially for the BCC graded lattice. The reason is that the β values provided in Figure A.7 (A.3) are obtained from the least square method in such a way that the total error between $(E/E_0)^{(k)}$ and $(E(x)/E_0)$ along the whole graded direction be minimized, which does not guaranty the best fitting for the inverses, particularly when the relative modulus is very low (the inverse is very high), as seen in the BCC lattice. Hence, one should notice that for the cases demanding the inverse of the function of relative modulus,

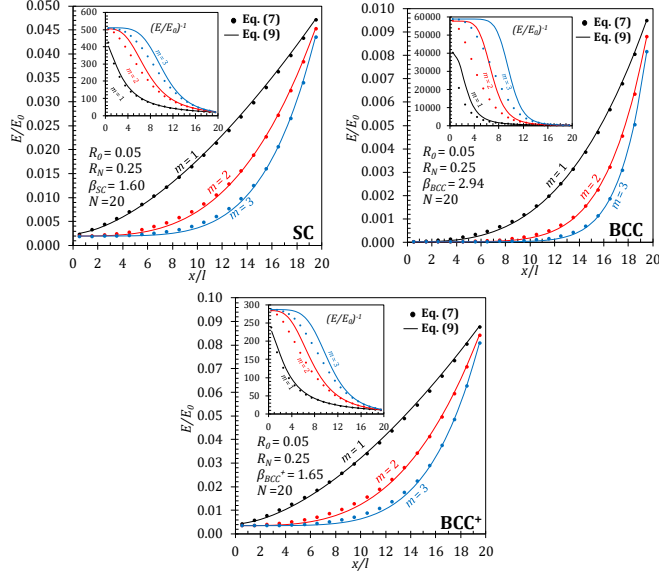


Figure 1.9. The variation of elastic modulus along the graded axis x and the accuracy test of the fitting function presented in Equation (1.9).

such as $(E(x)/E_0)^{-1}$ in Equation (1.16), another curve fitting with the values of inverse relative modulus as the input is needed to be performed to look for the updated values of the β parameter which are exclusively fitted on the inverse values.

Then, the coefficient $C^{(0)}$ and $n^{(0)}$ of the classical Gibson-Ashby model for the *uniform* SC, BCC, and BCC⁺ lattices are obtained by fitting Equation (1.19) to the relative elastic modulus and relative densities of uniform lattices presented in Equation (1.4) and Equation (1.8), respectively. Figure 1.10 depicts the output of the fitting and the corresponding calibrated coefficients. Note that the uniform dimensionless diameter, R , varies in the range of $0.05 < R < 0.5$ for both SC and BCC lattices resulting in a relative density range of $0.0057 < (\rho/\rho_0)_{SC}^{(0)} < 0.412$ and $0.013 < (\rho/\rho_0)_{BCC}^{(0)} < 0.748$. However, the range for the BCC⁺ lattice is limited to $0.05 < R < 0.4$ corresponding to the relative density range of $0.018 < (\rho/\rho_0)_{BCC^+}^{(0)} < 0.694$ to avoid a very high relative density of 0.869 for $R = 0.5$. A precise fitting of the power law Gibson-Ashby equation on the plot of analytical relative modulus versus relative density is observed, as expected. One should pay attention that the correction factor, $\gamma < 1$ introduced in Equation (1.5), is applied to the calculated relative densities in Figure 1.10, and it is the reason why the calibrated values differ from the approximated ones with $\gamma = 1$, for example, $C^{(0)} = 1/3$ and $n^{(0)} = 1$ for the uniform SC lattice by simply comparing Equation (1.4a) and Equation (1.8a) (See [28]).

Besides, in Figure 1.10 the relative elastic modulus obtained from FE-UC sim-

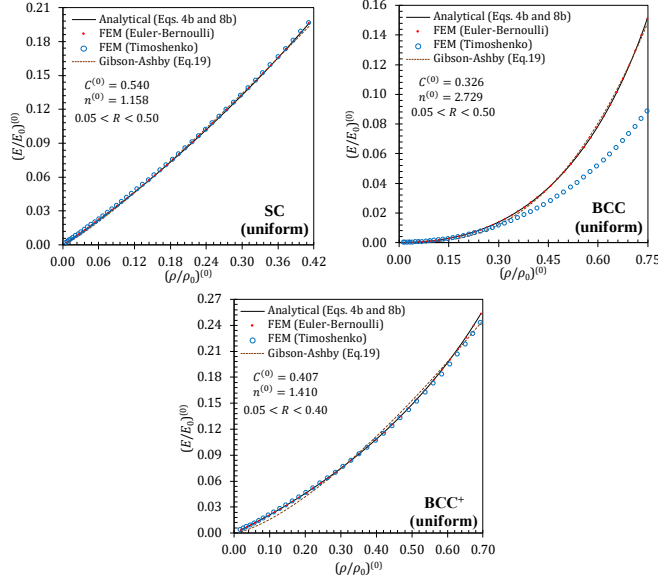


Figure 1.10. The relative elastic modulus versus the relative density and the calibrated Gibson-Ashby model for the uniform lattices.

ulations based on both the Euler-Bernoulli and the Timoshenko beam theories are depicted. The Euler-Bernoulli remarkably fits the analytical prediction which confirms the correctness of the exact expression derived from the same theory, while the Timoshenko predicts lower elastic modulus for BCC and BCC⁺ lattices where the shear deformations play a role, particularly for BCC with all the ligaments inclined. The shear deformation effect grows by increasing R (thicker ligaments).

After that, the capability of the modified Gibson-Ashby model (Equation (1.20)) in relating the effective relative modulus to the effective relative density and the accuracy of the correction factor, κ presented in A.5, is examined in Figure 1.11, Figure 1.12, and Figure 1.13 for SC, BCC, and BCC⁺ graded lattices, respectively. For each lattice, three cases of graded changes are inspected: The first two cases consider a high (400%, $(R_N/R_0 = 5)$) variation in the diameter of ligaments with $m = 1$ and $m = 3$ to also reveal the effect of power, while the last case assumes a lower (200% $(R_N/R_0 = 3)$) linear ($m = 1$) change in the diameters of ligaments along the graded direction. In all cases, the effective relative density is increased by increasing both R_0 and R_N proportionally to keep constant their ratio. The minimum of R_0 is 0.05 while the maximum of R_N is 0.5 for SC and BCC, and 0.4 for BCC⁺ to avoid too high local relative densities (see the ranges of R_0 and R_N mentioned in the graphs). The exact values of effective elastic modulus given by Equation (1.10) are plotted versus the exact values of effective relative density Equation (1.15) and the corresponding effective relative elastic modulus predicted by the classical (Figure 1.10) and the mod-

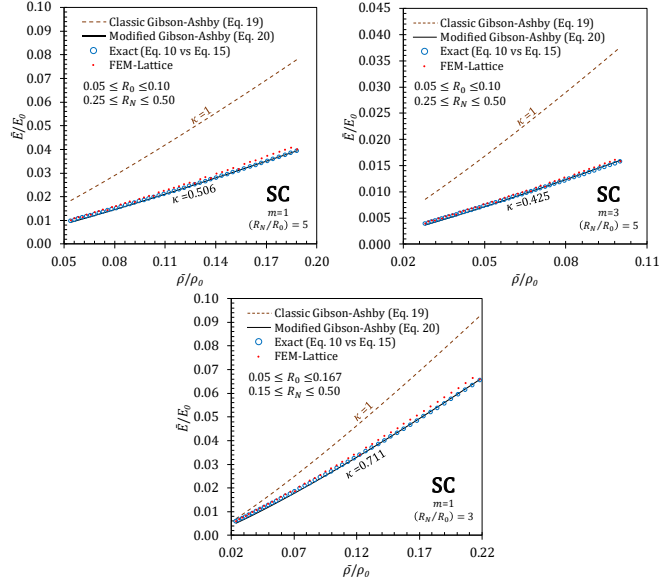


Figure 1.11. The effective relative elastic modulus, $\bar{E}/E_0$, versus the effective relative density, $\bar{\rho}/\rho_0$ for the SC graded lattice.

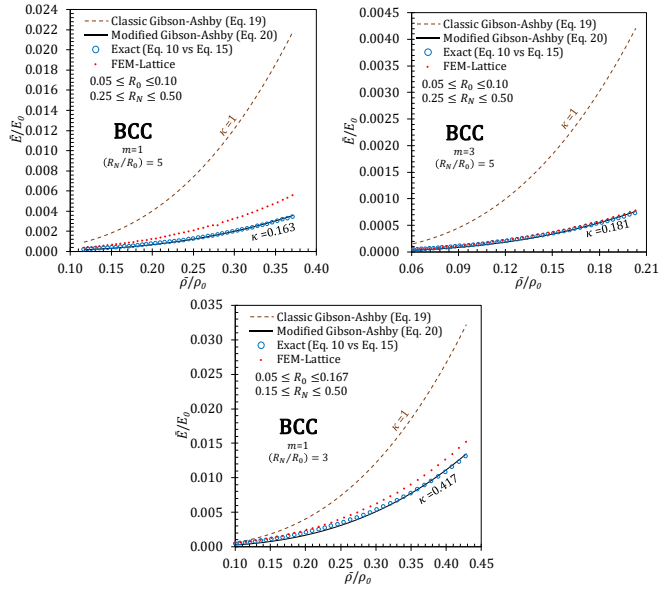


Figure 1.12. The effective relative elastic modulus, $\bar{E}/E_0$, versus the effective relative density, $\bar{\rho}/\rho_0$ for the BCC graded lattice.

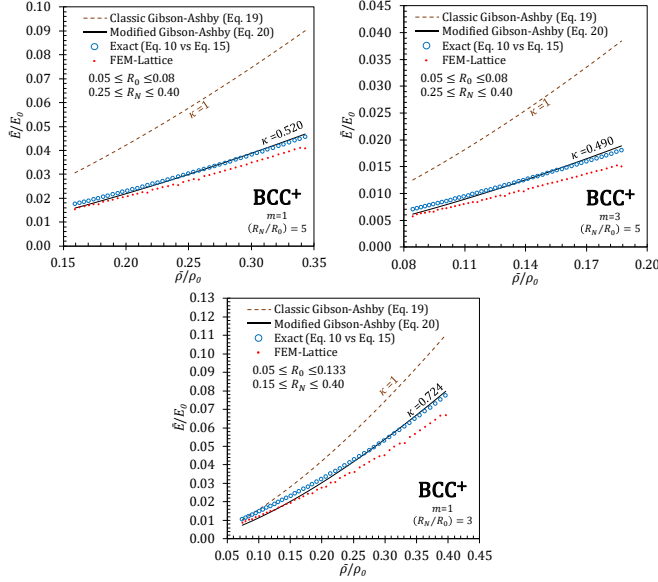


Figure 1.13. The effective relative elastic modulus, $\bar{E}/E_0$, versus the effective relative density, $\bar{\rho}/\rho_0$ for the BCC⁺ graded lattice.

ified (Equation (1.20)) Gibson-Ashby models are plotted. First, it is proved that the classical model with the coefficients obtained from the fitting to the uniform lattices is not able to predict accurately the relationship between the effective properties of graded lattices. One can observe from Figure A.14 that increasing the graded ratio, (R_N/R_0) , causes the correction factor, κ , to be further away from the value of one, $\kappa=1$, which means that the error between the original Gibson-Ashby model and the effective properties of the graded lattice structure is increasing. Accordingly, the error increases dramatically comparing the high graded ratio of $(R_N/R_0) = 3$ to the lower ratio $(R_N/R_0) = 3$. Second, it is confirmed that the calibrated correction factor, κ , is able to fit accurately the exact effective properties for all nine samples. Note that the calibrated correction factor of graded lattices is always lower than one, $\kappa < 1$, which rectifies the overestimation of the effective elastic modulus by the classical model with $\kappa = 1$ which is the worst for the BCC lattice. In addition, the results obtained from FE-Lattice simulations introduced in Section 1.2.6 are plotted in Figure 1.11, Figure 1.12, and Figure 1.13. These numerical simulations are close to the predictions of the modified Gibson-Ashby model which approves the need of introducing the modification into the classical model.

Finally, the question raised in Section 1.2.5, i.e., "Which of the classical or the modified Gibson-Ashby models fit better the local (cell by cell) relative modulus to the local relative density?" is answered. The variation of the local relative elastic modulus, $E(x)/E_0$, versus the local relative density, $\rho(x)/\rho_0$, both evaluated from

Equation (1.9), are compared to the local relative modulus predicted by the classical (Equation (1.22)) and the modified (Equation (1.23)) local Gibson-Ashby models in Figure 1.14, Figure 1.15, and Figure 1.16 for SC, BCC, and BCC⁺ graded lattices, respectively. Three cases of study for each lattice are performed which indeed

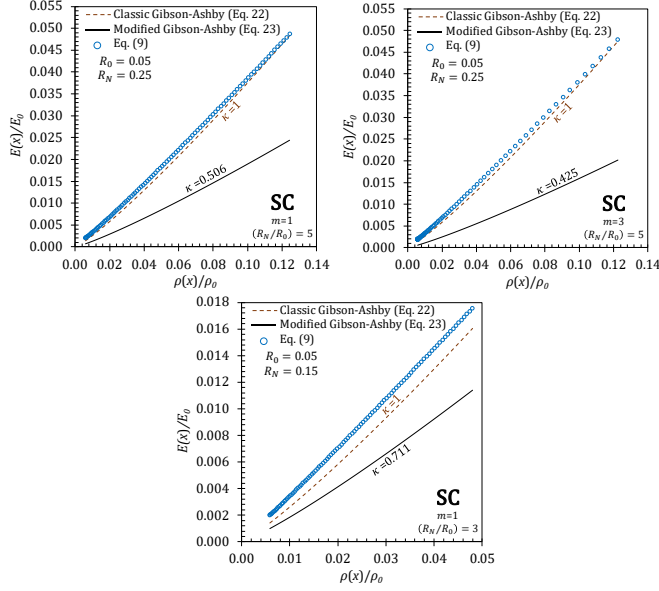


Figure 1.14. The local (cell by cell) relative elastic modulus, $E(x)/E_0$, versus relative density, $\rho(x)/\rho_0$ for the SC graded lattice.

expand the first point of the plots in Figure 1.11, Figure 1.12, and Figure 1.13) along the graded direction, x (see the values of R_0 and R_N mentioned in the graphs). It is seen that the classical formulation $\kappa = 1$ is more accurate from the local point of view compared to the modified version calibrated using the overall effective properties. This is because, locally, each unit cell has almost a uniform structure, and therefore $\kappa = 1$ can better relate the properties cell by cell. Similar to the effective properties, the worst prediction of the classic and modified models belongs to the BCC lattice.

1.3.2 Experimental results

A set of experiments was performed to validate the analytical formulations derived in the previous section. The samples to be tested were printed by a Stratasys J750TM 3D printer using high-quality mode setting (resolution of $27\mu\text{m}$ layer height and dimensional accuracy of $200\mu\text{m}$). A 3D printer exploiting a material-jetting technology was used since it allows obtaining almost isotropic samples with relatively small defects [10]. A single configuration for each one of the considered unit cells was printed, namely a SC, BCC, and BCC⁺. While the length of the unit cell is $l = 16$ mm, the

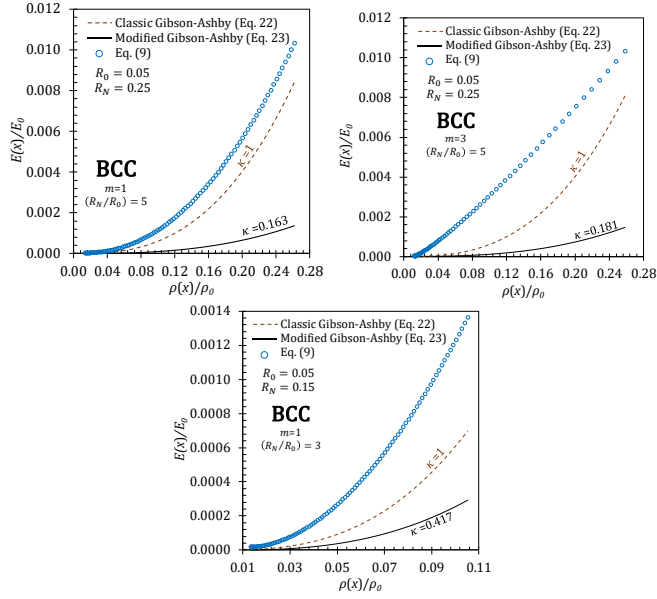


Figure 1.15. The local (cell by cell) relative elastic modulus, $E(x)/E_0$, versus relative density, $\rho(x)/\rho_0$ for the BCC graded lattice.

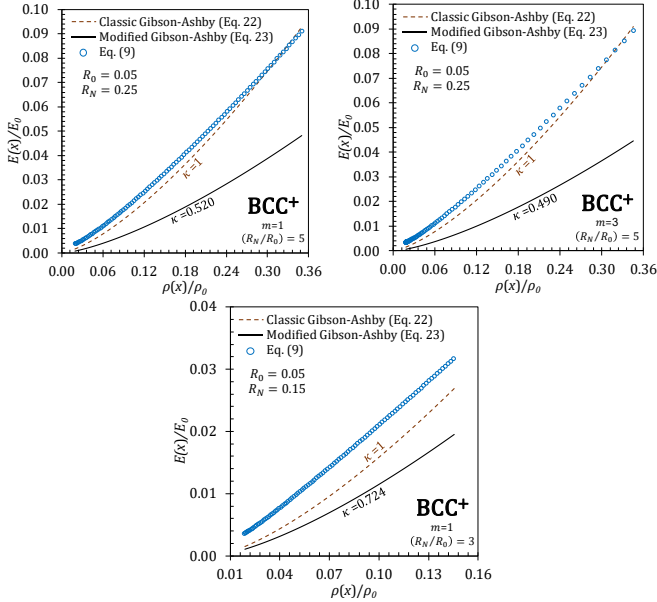


Figure 1.16. The local (cell by cell) relative elastic modulus, $E(x)/E_0$, versus relative density, $\rho(x)/\rho_0$ for the BCC⁺ graded lattice.

$R_0 = 0.125$ and the $R_N = 0.375$ i.e. $d_0 = 2\text{mm}$ and $d_N = 6\text{mm}$. The printed samples are shown in Figure 1.17. It is worth mentioning that for the experimental models, $m = 1$ for all the models.

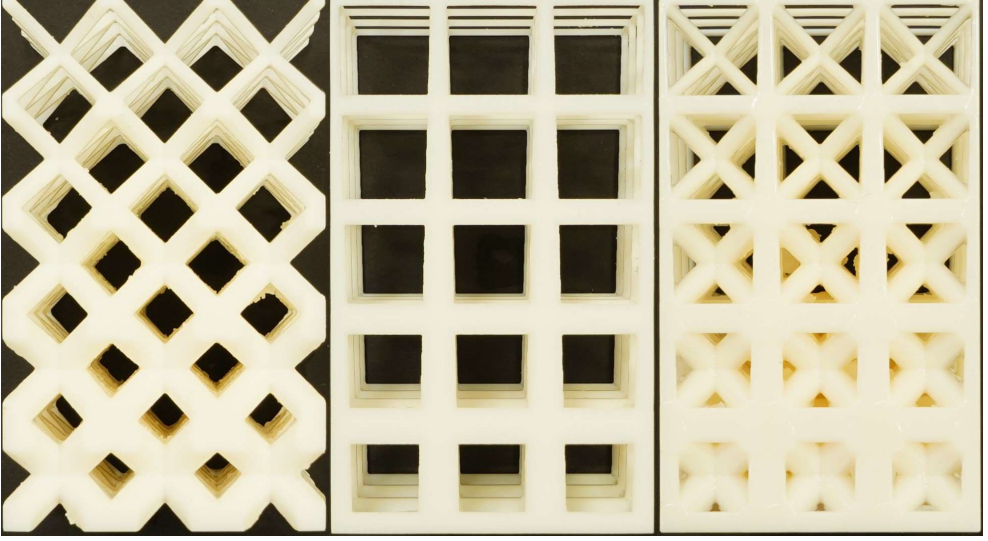


Figure 1.17. The printed functionally graded lattice structure samples that were tested under compression loading. Right: BCC, center: SC and left: BCC⁺

All samples were printed in Vero PureWhite™ material whose mechanical properties were estimated by specific uniaxial testing accordingly with ASTM-D638 (see Figure 1.18). To perform these auxiliary tests, a constant strain rate of 0.1 mm/sec was imposed on the top cross-head of the loading frame machine (BETA 100 by MESSPHYSIK). From these tests, an average elastic modulus of $E_0 = 1436 \pm 10$ MPa has been estimated. A density $\rho_0 = 1.175\text{g/cm}^3$ has been estimated for the bulk material.

To evaluate the effective elastic modulus of the 3D printed FG lattice structures, compression tests were conducted by imposing a constant strain rate of 0.1 mm/sec to the top face of the samples with a BETA 100 loading frame machine. Three tests were performed for each configuration, following ASTM-D638 standards. Prior to performing such compression tests, all the FG lattices were weighted to estimate their relative density ($\bar{\rho}/\rho_0$) which is reported in Table 1.1. As can be seen from the results reported in this table, the correction factor γ in Equation (1.4) allows to predict the relative density of the FG lattice structures with good accuracy as it excludes from the calculation of the overlapped volumes in the joints.

A comparison of the relative effective elastic modulus ($\bar{E} / E_0$) obtained from the experiments with those obtained by the analytical model is shown in Table 1.2. It is noteworthy that the experimental tests exhibit minimal data scatter, with standard variations less than ± 5 in all cases. The reported relative elastic modulus values



Figure 1.18. The fabricated dog-bone samples uni-axially tested to estimate the mechanical properties of the bulk material (Vero PureWhite™) used to print the FG lattice structures.

Table 1.1. Evaluated relative density ($\bar{\rho}/\rho_0$) from the experimental tests and the corresponding analytical estimation

	SC	BCC	BCC+
Exact (Equation (1.4), $\gamma < 1$)	0.131	0.272	0.358
Experimental	0.145 ± 0.002	0.299 ± 0.014	0.394 ± 0.018
Approximate (Equation (1.4), $\gamma = 1$)	0.160	0.367	0.527

are the average of the three experimental data, demonstrating the reliability of the

current approach for modifying the Gibson-Ashby model.

Table 1.2. Evaluated relative effective modulus ($\bar{E} / E_0$) from the experimental tests and the corresponding analytical results

	SC	BCC	BCC+
Exact (Equation (1.15))	0.0368	0.0075	0.0687
Experiments	0.0396 ± 0.0017	0.0062 ± 0.0003	0.0703 ± 0.0031
Modified Gibson-Ashby (Equation (1.20))	0.0364	0.0069	0.0725
Classic Gibson-Ashby (Equation (1.19))	0.0520	0.0093	0.0870

1.4 Conclusion

In this paper, a novel analytical framework for evaluating the mechanical properties of functionally graded lattices is developed where the relative density and consequently the relative elastic modulus vary along the graded direction due to gradual changes in the diameters of ligaments keeping constant the lattice parameter as a repetitive non-homogeneous structure. Three common cubic lattice systems, i.e., simple cubic (SC), body-centered cubic (BCC), and their combination (BCC⁺) are chosen as the geometry of unit cells. The first level of homogenization is accomplished by deriving an exact expression for the relative density and the relative elastic modulus of the k th cell along the graded direction performing a structural analysis of the representative beam frame of the unit cell including tapered beams. For ease of use in practical applications, continuous functions that approximate the variation of relative density and relative elastic modulus along the graded direction are introduced and fitted to the exact expressions at the center of cells via a least square approach in a broad range of changes in the geometry of the graded lattice. As the second level of homogenization, the exact expression for the effective relative density and the effective relative elastic modulus are derived to convert the graded lattice to a fully homogenized equivalent solid.

The modified Gibson-Ashby model is suggested to relate the effective relative modulus to the effective relative density of graded lattice by introducing a correction factor to the original equation since it is shown that the coefficients fitted to the uniform lattices can not accurately fit the effective properties. The calibrated correction factor is presented for a wide range of possible geometries of the graded lattices in graphical form as well as approximated equations for the three lattices. Furthermore, it is proved that the classical model calibrated to uniform structures is able to match the local (cell by cell) relative elastic modulus to the local relative density along the graded direction. It suggests an practical, easy-to-use framework for designing optimized graded lattice structures avoiding high-cost simulations and/or experimental measurements.

CHAPTER 2

A Refined Gibson-Ashby Model for Functionally Graded Honeycombs with Random Irregularities

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To be submitted in a Q1 high ranked journal

Abstract: This study refines the Gibson-Ashby equation for predicting the elastic modulus of honeycombs by introducing two correction factors, κ and η , accounting for functionally graded (FG) wall thickness variations and random irregularities, respectively, i.e., $(\text{relative modulus}) = \kappa\eta C (\text{relative density})^n$. Analytical expressions based on Timoshenko beam theory are extended to FG architectures, providing a stepwise formulation for relative density and elastic modulus variations along the FG direction. This yields a closed-form expression for the effective relative elastic modulus of FG honeycombs, validated by finite element (FE) simulations. Here, κ is calibrated over a broad range of linear and nonlinear wall thickness gradients. Since closed-form formulations for periodic lattices cannot capture random irregularities, η is fitted to an extensive set of FE simulations with random designs. These correction factors are presented as design charts covering hexagonal, square, and triangular honeycombs. Model accuracy is validated against 3D-printed samples, demonstrating its capability to predict elastic modulus reduction with precision. The framework thus enables straightforward estimation of the elastic modulus of irregular FG honeycombs, bridging analytical models and real-world imperfections. Designers can apply these factors to predict grading and randomness effects without relying on extensive testing, providing a practical tool for optimizing graded architected materials.

Highlights:

- Functionally graded honeycombs with a random irregularity are parameterized.
- Exact expression for effective relative elastic modulus is reported
- The classical Gibson-Ashby model is modified to account for graded variation and irregularity.
- FE numerical simulations are conducted.
- Compression tests are performed on 3D-printed samples.

keywords: Functionally Graded, Gibson-Ashby Model, Irregular Lattice structures, Porosity, Honeycombs, Additive manufacturing.

2.1 Introduction

Recent advances in digital and additive manufacturing have significantly expanded the design space for cellular solids, enabling the fabrication of complex architectures with tailored properties [48]. Cellular solids encompass a broad class of engineered porous materials. Honeycombs, a subset of cellular solids, are commonly formed by in-plane repetition of a two-dimensional unit cell with extrusion along the third dimension [11]. Conventional honeycomb designs with hexagonal, triangular, and square unit cells, have been widely studied due to their well-defined periodicity, which simplifies both manufacturing and modeling [49]. However, non-periodic and irregular honeycomb architectures—where structural variations arise from graded wall thickness or random irregularities in unit cell geometry—have received significantly less attention despite their potential advantages. Natural systems, such as bones, frequently exploit both graded and irregular architectures to enhance mechanical efficiency, motivating the exploration of such designs for engineered structures. Expanding beyond conventional periodic designs allows for optimized honeycombs with superior mechanical performance [50], particularly in lightweight applications such as aerospace and automotive engineering, as well as biomedical applications [51]. Historically, the fabrication of non-periodic structures was constrained by manufacturing limitations, leading to a preference for uniform, periodic honeycombs. However, recent developments in additive manufacturing have overcome these constraints, enabling precise control over spatial variations in geometry and unlocking new opportunities for functional grading (FG) and random irregularity in honeycombs [50, 52].

For periodic cellular solids with a well-defined repeating unit cell, the relationship between mechanical properties and relative density can be derived through structural mechanics analysis [16–18, 30, 53–59]. Under simplified assumptions, the structural analysis may result in a closed-form expression similar to the power-law form of the classical Gibson-Ashby equation [11], where a mechanical property is evaluated as $C \times (\text{relative density})^n$. In such cases, direct comparison with analytical solutions allows for the determination of multiplier C and exponent n . However, when the simplified assumptions in structural mechanics analysis break down—such as in cases where the wall thickness-to-length ratio is large and shear-axial-bending coupling happens and the walls’ overlaps in joints are not ignorable—the analytically derived equations (if exist) may not obey the simplified classical power-law form of the Gibson-Ashby equation. In these scenarios, the classical Gibson-Ashby equation is not able to accurately fit experimental and/or FE simulation results over a wide range of relative densities. Besides, when the structure lacks periodicity, the power-law equation may be empirically fitted to the data to obtain the most suitable values for C and n [19]. In some cases, the classical Gibson-Ashby power-law form fails to provide a reliable best-

fit across a broad density range, necessitating modifications to the original form [60].

Given the effectiveness of FG microstructures, numerous studies have explored their potential to enhance the mechanical performance of cellular solids. The fundamental concept behind FG design is to introduce a controlled variation in microstructural parameters—such as cell wall thickness, pore size, or bulk material—to achieve optimized mechanical behavior. Compared to repetitive uniform structures, FG configurations offer significant advantages in tailored mechanical responses owing to functional material distribution [61]. Key investigations have demonstrated that FG designs can substantially improve kinetic energy absorption [62–65], reduce initial peak stress under impact loading [66], and enhance buckling collapse [67]. These findings make FG designs highly promising for various engineering applications from graded scaffolds [68–71] to microwave lenses [72].

The application of FG cellular solids as structural components, such as beams and plates, has been widely investigated. These studies have demonstrated how a controlled distribution of material along the thickness or length of a structural element can effectively tailor its mechanical response such as stability [73–75], and vibrations [33, 34, 76, 77], ultimately leading to optimized structural designs. In such configurations, the mechanical properties vary spatially, making the structure inherently heterogeneous. The foundational approach in most of these studies relies on the Gibson–Ashby equation to establish a relationship between the relative density distribution and the corresponding variations in elastic properties within the structure [32, 35]. However, a review of the literature indicates that in some cases, applying the Gibson–Ashby relation to define property variations within an FG cellular structure, based on spatial coordinates, has led to misunderstandings and misinterpretations by researchers [31]. This highlights the necessity for further investigations into the applicability and limitations of the Gibson–Ashby equation for FG cellular solids, ensuring its accurate use in structural modeling and optimization.

The study of random irregularities in honeycomb structures has been relatively limited, primarily due to the challenges associated with extending analytical formulations for periodic models to irregular, stochastic architectures. From an experimental standpoint, investigating the effects of random irregularities requires testing a large set of samples to capture the statistical distribution of structural imperfections, which can be costly and time-consuming. FE simulations have been employed as a practical alternative to reduce experimental costs while systematically analyzing the influence of randomness on mechanical properties. Findings indicate that by adjusting the degree of irregularity, it is possible to tailor mechanical performance for a given relative density. This offers a promising avenue for optimizing lattice structures where mechanical behavior can be fine-tuned without altering the overall material volume fraction [62, 78–81].

This study directly addresses a critical gap in extending the classical Gibson–Ashby model to FG and randomly irregular honeycombs. A fundamental question in cellular solid design is whether the same power-law exponent n and multiplier C , calibrated for uniform periodic honeycombs, remain valid for FG and irregular architectures. Our findings demonstrate that applying the classical Gibson–Ashby equation

without modification leads to significant errors in predicting the elastic modulus of such structures. However, we show that by introducing two correction factors— κ to account for FG variations and η to capture random irregularities—the classical framework can still provide accurate predictions without altering the exponent n . To facilitate practical implementation, κ and η are systematically calibrated through a combination of analytical modeling and extensive FE simulations, covering a wide spectrum of FG profiles (both linear and nonlinear) and degrees of randomness. The results are presented in the form of design charts, for conventional honeycomb designs namely, hexagonal (HEX), triangular (TRI), and square (SQ), offering a straightforward tool for engineers to optimize FG irregular honeycombs while leveraging existing knowledge of uniform periodic architectures. By bridging the gap between theoretical models and real-world applications, this work provides an innovative and practical methodology for integrating FG and irregular lattice structures into advanced structural designs.

2.2 Development of the Model

2.2.1 Defining the geometry of FG honeycombs

Three different conventional unit cells have been selected for analysis i.e. HEX, TRI, and SQ [11]. Before introducing any random irregularities, the unit cells are assumed to be regular polygons with equal wall lengths of l , as shown in Figure 2.1. Note that for TRI and SQ lattices, the unit cell length is $a = l$ while for HEX it is $a = \sqrt{3}l$.

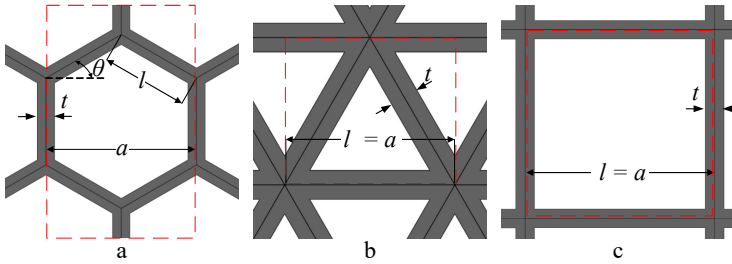


Figure 2.1. Three different unit cells with their geometrical parameters a) hexagonal (HEX), b) triangular (TRI), and c) square (SQ) unit cell.

There are three ways to achieve a graded honeycomb structure. The first is by gradually changing the properties of the bulk material while keeping the honeycomb geometry unchanged. The second is by gradually changing the honeycomb wall length, while keeping the bulk material, and wall thickness fixed. The third is by gradually changing the thickness of the walls while keeping the bulk material, and honeycomb constant (constant unit cell length) fixed. Here, the third method is chosen because the first method encounters limitations in multi-material fabrication, while the second

method introduces inevitable irregularities in the honeycomb structure, akin to the variations in pore size observed in irregular foams.

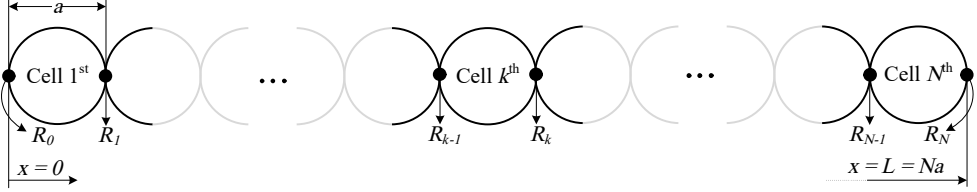


Figure 2.2. The schematic of the graded honeycomb structure across FG direction, x . The dimensionless aspect ratio of the k th unit cell is the average of the aspect ratio of walls at the nodes on both sides.

According to Figure 2.2, a honeycomb structure with N unit cells of length a , and a total length of $L = Na$ has been assumed in which the thickness of walls located in the i th node between the cells has a certain thickness of t_i . The dimensionless thickness (aspect ratio) of the wall at the i th node can be defined as $R_i = t_i/l$. In order to introduce the graded functionality to the honeycomb structure, the aspect ratio can be changed from R_0 at $x = 0$ to R_N at $x = L$ and the function of gradation is assumed as:

$$R_i = R_0 + \Delta R \left(\frac{i}{N} \right)^m, \quad (2.1)$$

in which $\Delta R = R_N - R_0$, and $i = 0, 1, 2, \dots, N$. Here, the exponent m is chosen to be 1, 2, or 3 to capture both linear ($m = 1$) and nonlinear ($m \neq 1$) changes in the gradient. This allows for the consideration of various behaviors associated with the gradation in this study. Next, the average aspect ratio within the k th cell, $\bar{R}_k$, is defined by averaging the value of R at the $(k-1)$ th, and k th nodes as,

$$\bar{R}_k = \frac{R_{k-1} + R_k}{2} = R_0 + \frac{\Delta R}{2N^m} ((k-1)^m + k^m), \quad (2.2)$$

where $k = 1, 2, \dots, N$. The elastic modulus of an FG honeycomb can be evaluated based on this step-wise variation of the aspect ratio through the length.

2.2.2 Relative density and elastic modulus of honeycombs

The relative density of a unit cell is a function of its constant aspect ratio, R , e.i., $\rho/\rho_0 = f(R)$, which can be evaluated by summing up the volume of all the walls within the unit cell divided to its total volume. However, the real relative density may be overestimated due to including the overlap part in the walls' joints which is higher for the bigger value of R . Excluding the overlaps in the joints, the exact value of the relative density for the honeycombs with HEX, TRI, and SQ unit cells can be

evaluated as follows [82–85]:

$$\left(\frac{\rho}{\rho_0}\right)_{HEX} = \frac{2}{\sqrt{3}}R - \frac{1}{3}R^2, \quad (2.3a)$$

$$\left(\frac{\rho}{\rho_0}\right)_{TRI} = 2\sqrt{3}R - 3R^2, \quad (2.3b)$$

$$\left(\frac{\rho}{\rho_0}\right)_{SQ} = 2R - R^2, \quad (2.3c)$$

where ρ_0 is the density of bulk material. Likewise, the relative elastic modulus of the unit cell is a function of its aspect ratio e.i. $E/E_0 = g(R)$. Employing structural analysis based on shear deformable Timoshenko beam theory, the relative elastic modulus for HEX, TRI, and SQ unit cells is calculated as follows [82–85]:

$$\left(\frac{E}{E_0}\right)_{HEX} = \frac{4R^3}{\sqrt{3}} \frac{1}{1 + (5.4 + 1.5\nu_0)R^2}, \quad (2.4a)$$

$$\left(\frac{E}{E_0}\right)_{TRI} = \frac{2R}{\sqrt{3}} \frac{1 + R^2}{1 + \frac{1}{3}R^2}, \quad (2.4b)$$

$$\left(\frac{E}{E_0}\right)_{SQ} = R, \quad (2.4c)$$

where E_0 and ν_0 are the elastic modulus and the Poisson's ratio of the bulk material. The relative density and elastic modulus of a uniform honeycomb with a fixed aspect ratio R_u is constant across the whole structure. They can be evaluated by setting $R = R_u$ in Equation (2.3) and Equation (2.4). By contrast, in the FG honeycombs the aspect ratio R varies from R_0 to R_N according to Equation (2.1). It results in a step-wise change along the FG direction, which is the x axis in this study. The relative density, $(\rho/\rho_0)^{(k)}$, of the k th unit cell of an FG honeycomb is calculated by substituting the average aspect ratio, $\bar{R}_k$, from Equation (2.2) to Equation (2.3):

$$\left(\frac{\rho}{\rho_0}\right)_{HEX}^{(k)} = \frac{2}{\sqrt{3}}\bar{R}_k - \frac{1}{3}\bar{R}_k^2, \quad (2.5a)$$

$$\left(\frac{\rho}{\rho_0}\right)_{TRI}^{(k)} = 2\sqrt{3}\bar{R}_k - 3\bar{R}_k^2, \quad (2.5b)$$

$$\left(\frac{\rho}{\rho_0}\right)_{SQ}^{(k)} = 2\bar{R}_k - \bar{R}_k^2. \quad (2.5c)$$

Similarly, the relative elastic modulus, $(E/E_0)^{(k)}$, is obtained by replacing R with $\bar{R}_k$ in Equation (2.4):

$$\left(\frac{E}{E_0}\right)_{HEX}^{(k)} = \frac{4\bar{R}_k^3}{\sqrt{3}} \frac{1}{1 + (5.4 + 1.5\nu_0)\bar{R}_k^2}, \quad (2.6a)$$

$$\left(\frac{E}{E_0}\right)_{TRI}^{(k)} = \frac{2\bar{R}_k}{\sqrt{3}} \frac{1 + \bar{R}_k^2}{1 + \frac{1}{3}\bar{R}_k^2}, \quad (2.6b)$$

$$\left(\frac{E}{E_0}\right)_{SQ}^{(k)} = \bar{R}_k. \quad (2.6c)$$

2.2.3 The approximation function for density and elastic modulus of FG honeycombs

Since the gradation of the aspect ratio is based on a power law with the exponent m (Equation (2.1)), given the values of relative density and elastic modulus of unit cells by Equation (2.5) and Equation (2.6), one may fit an approximation function of the form $Ax^{\alpha m} + B$ on these values along the FG direction, x , as,

$$P(x) \approx Ax^{\alpha m} + B, \quad (2.7a)$$

$$A = \frac{P^{(N)} - P^{(1)}}{a^{\alpha m}((N - 0.5)^{\alpha m} - 0.5^{\alpha m})}, \quad (2.7b)$$

$$B = P^{(1)} - (0.5a)^{\alpha m} A, \quad (2.7c)$$

in which $P(x)$ is either relative density or relative elastic modulus ($\rho(x)/\rho_0$ or $E(x)/E_0$) and α is a calibrated parameter which can be evaluated by use of curve fitting method, illustrated in Figure B.1 and Figure B.2 in **Supplementary Information File** for different geometries. The calibrated parameter α has been calculated for a range of $R_0 < R_N < 0.5$. Note that during the fitting of $P(x)$, the properties of cells are assigned to their central x -coordinates. Besides, Equation (2.7) is fitted so that it exactly passes through the relative properties of the first ($k = 1$) and the last ($k = N$) unit cell which are evaluated at $x = 0.5a$ and $x = (N - 0.5)a$, respectively. Given Equation (2.7), it is possible to approximate a discontinuous FG honeycomb structure as a continuous graded medium. Figure B.3 and Figure B.4 in **Supplementary Information File** plot fitted approximation functions, Equation (2.7) for relative density and elastic modulus, by setting $N = 20$ and considering a wide range of variation in wall aspect ratio, ranging from 0.05 to $R = 0.25$, while the corresponding calibrating parameter, α , is evaluated from the graphs in Figure B.1 and Figure B.2 in **Supplementary Information File**. Furthermore, to expand the range of grading variation in aspect ratio, three values of $m = 1, 2$, and 3 are also considered. Figure B.3 and Figure B.4, confirm the accuracy of the approximated

functions introduced in Equation (2.7). It is important to note that the fitting parameter α for the relative modulus of the honeycomb with a SQ unit cell is equal to 1, as indicated by Equation (2.4c).

2.2.4 The effective properties of FG honeycombs

In the next step of homogenization, the FG honeycombs can be treated as a fully homogeneous medium by introducing *effective* properties denoted by a bar ($\bar{\cdot}$). The effective density $\bar{\rho}$ can be described as the density of a fully homogeneous material whose mass is the same as the total mass of FG honeycombs with N cells while they have an identical apparent volume of $Na hb$ in which hb is the unit cell cross-section area perpendicular to the FG direction. The effective density can be evaluated as the average of the cells' density:

$$\frac{\bar{\rho}}{\rho_0} = \frac{1}{N} \sum_{k=1}^N \left(\frac{\rho}{\rho_0} \right)^{(k)}. \quad (2.8)$$

However, using the continuous approximation form of the graded relative density, Equation (2.7), converts the summation to an integration form:

$$\frac{\bar{\rho}}{\rho_0} \approx \frac{\int_0^{Na} \left(\frac{\rho(x)}{\rho_0} \right) dx}{Na} = \frac{A(Na)^{(\alpha m)}}{\alpha m + 1} + B. \quad (2.9)$$

The FG honeycombs can be considered as N unit cells with the elastic modulus of $E^{(k)}$, $k = 1, \dots, N$ which are connecting in series. The total elongation of the FG honeycombs under an applied load F_x is:

$$\delta_{graded} = \frac{F_x a}{hb} \sum_{k=1}^N \frac{1}{E^{(k)}}, \quad (2.10)$$

while the elongation of the equivalent fully homogeneous medium with a total length of Na is:

$$\bar{\delta} = \frac{F_x Na}{hb \bar{E}}. \quad (2.11)$$

Comparing Equation (2.10) and Equation (2.11) one can define the effective relative elastic modulus as:

$$\frac{\bar{E}}{E_0} = \frac{N}{\sum_{k=1}^N \frac{1}{(E/E_0)^{(k)}}}, \quad (2.12)$$

where $(E/E_0)^{(k)}$ is calculated from Equation (2.6). Similarly, the integration form related to the continuous approximated expression, Equation (2.7), can be written as,

$$\frac{\bar{E}}{E_0} \approx \frac{Na}{\int_0^{Na} \frac{1}{(E(x)/E_0)} dx}. \quad (2.13)$$

Note that replacing Equation (2.7) into Equation (2.13) may need a numerical integration. The values of effective relative density and effective elastic modulus respectively calculated from Equation (2.8) and Equation (2.12) have been illustrated in Figure B.5 to Figure B.7 in **Supplementary Information File** for a range of R_0 and R_N .

2.2.5 Definition of random irregularity

Various methods for introducing irregularity in honeycomb structures have been discussed in previous literature [62, 80, 81, 86–88]. For the current study, the following equations have been applied to the initial coordinates of each node of the regular configuration $(x_{regular}, y_{regular})$ to find the updated coordinate $(x_{irregular}, y_{irregular})$ corresponding to the irregular structure:

$$\begin{aligned} x_{irregular} &= x_{regular} + \Lambda_1 \Delta l \cos(2\pi\Lambda_2) \\ y_{irregular} &= y_{regular} + \Lambda_1 \Delta l \sin(2\pi\Lambda_2), \end{aligned} \quad (2.14)$$

in which $0 \leq (\Lambda_1 \text{ and } \Lambda_2) \leq 1$ represent random numbers, and Δ defines the degree

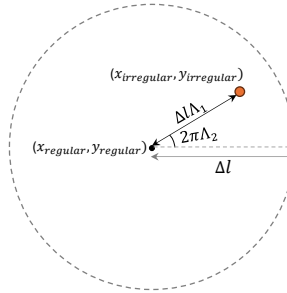


Figure 2.3. Definition of random irregularity in honeycombs. By setting to random parameters, Λ_1 and Λ_2 , the joint node relocates from its location in regular lattice to a random location within a circle of radius Δ (degree of irregularity).

of irregularity in the honeycomb structure. By applying Equation (2.14), each node of the regular structure is randomly relocated within a circle with the radius Δl , as illustrated in Figure 2.3. It is noteworthy that $\Delta = 0.5$ is the extreme value of the degree of randomness where there is a chance that some nodes may coincide, resulting in the removal of a wall from a unit cell. To maintain the number of walls in each unit cell, the maximum value of the randomness parameter is changing in the range of $0 \leq \Delta < 0.5$. Figure 2.4 illustrates two different degrees of randomness ($\Delta=0.25$

and 0.5) for the honeycombs. The degree of irregularity, denoted as Δ , can influence the elastic modulus, and its impact is incorporated into the modified Gibson-Ashby equation in Section 2.2.6 using the correction factor η .

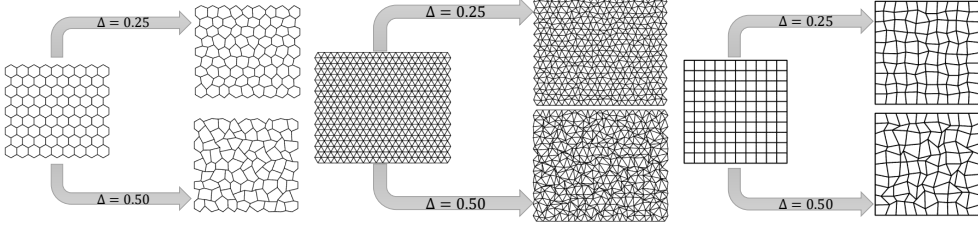


Figure 2.4. Regular and irregular HEX, TRI, and SQ honeycomb structures.
The degree of irregularity is controlled by varying Δ in the degree of 0 to 0.5.

2.2.6 Modified Gibson-Ashby model for FG irregular honeycombs

The standard Gibson-Ashby equation for a uniform honeycomb can relate the relative density and the relative elastic modulus as follows:

$$\frac{E_u}{E_0} = C \left(\frac{\rho_u}{\rho_0} \right)^n \quad (2.15)$$

in which C and n are defined as calibration parameters for a uniform honeycomb that should be fitted for a desired configuration. We propose the modified Gibson-Ashby model for FG honeycombs with a random irregularity by substituting Equation (2.8) and Equation (2.12) into Equation (2.15) and introducing κ and η as the correction factors for FG and random irregularity effects, respectively,

$$\frac{\bar{E}}{E_0} = \kappa \eta C \left(\frac{\bar{\rho}}{\rho_0} \right)^n \quad (2.16)$$

Accordingly, κ is a function f_1 of the degree of gradual changes in the wall thickness, controlled by the ratio (R_N/R_0) and the exponent m , while η is a function f_2 of the degree of randomness, Δ :

$$\kappa = f_1((R_N/R_0), m), \quad (2.17a)$$

$$\eta = f_2(\Delta), \quad (2.17b)$$

For the special case of $R_N/R_0 = 1$ or/and $m = 1$, the FG effect disappears, leading to a uniform honeycomb with $\kappa=1$. Besides, $\Delta = 0$ eliminates random irregularity resulting in $\eta=1$. The correction factor κ and η introduced here are later calibrated in Section 2.4 across a wide range of geometries for HEX, TRI, and SQ honeycombs.

Since the relative properties of the FG honeycombs vary in the gradation direction, x , based on the Equation (2.7), it makes sense to define the localized (cell by cell) version of the Gibson-Ashby equation. In order to evaluate the local relative properties, the FG correction factor is set to one ($\kappa=1$) in Equation (2.16), because within each cell the aspect ratio is almost uniform. Thus, the localized form is obtained as,

$$\frac{E(x)}{E_0} = \eta C \left(\frac{\rho(x)}{\rho_0} \right)^n \quad (2.18)$$

2.2.7 FE simulations

Numerical simulations using FE analysis have been conducted with the aid of the commercial software, COMSOL Multiphysics®. Three types of FE models have been utilized as follows:

- **2D beam model:** Each wall is defined as a beam with a rectangular cross-section. The out-of-plane depth is assumed to be equal to the wall length. For uniform configurations, the in-plane beam thickness is set based on the given aspect ratio, R_u , while for the FG honeycombs the beam thickness is defined as a function of x coordinate (FG direction) so that the aspect ratio varies from the given R_0 and R_N at two sides with a power of m . For irregular models, the joints are randomly relocated based on Equation (2.14). A unit cell count of $N=20$ along both in-plane directions has been defined to ensure independence from the number of unit cells, alongside the previous literature [84]. The convergence studies for the unit cell number have been detailed in Figure B.8 in **Supplementary Information File**. Each beam is discretized to 10 Timoshenko beam elements with a cubic displacement field and a quadratic rotation field. Our convergence study confirms that for 10 elements per beam, the calculated relative elastic modulus accurately converges. A sample meshed model for a uniform TRI geometry is presented in Figure B.13 in **Supplementary Information File**. This 2D beam model is used for three purposes in this study: first, the validation study of the model in Figure 2.6 and Figure 2.7. Second, calibration of the random irregularity correction factor η , i.e., FE results in Figure B.11 in **Supplementary Information File**. Third, the comparison study for the validity of correction factors, i.e., FEM Beam in Figure 2.9. In the third case, the geometry of the model is identical to the 3D-printed samples while the walls are modeled as beam elements.
- **2D plane-stress solid model:** The 2D sketch of CAD models of 3D-printed samples (before extrusion) are used as the geometry without any modifications. The out-of-plane thickness is set to 10 mm identical to 3D-printed samples and a plane-stress condition is applied. Models are meshed by a Free triangular element with a quadratic serendipity displacement field. The convergence study is presented in Figure B.12, indicating that the calculated relative modulus converges rapidly by increasing the number of elements. An "extra fine"

mesh resolution is applied to all models in COMSOL Multiphysics®. A sample meshed model of an FG-regular HEX geometry is presented in Figure B.13 in **Supplementary Information File**. The results of this FE model are solely reported in Figure 2.9, as FEM Solid 2D, for the comparison study.

- **3D structural solid model:** The 3D CAD models of 3D-printed samples are used as the geometry without any modifications. The models are meshed by a Free tetrahedral element with a quadratic serendipity displacement field. An "extra fine" mesh resolution is applied to all models in COMSOL Multiphysics®. A sample meshed model of an FG-irregular SQ geometry is presented in Figure B.13 in **Supplementary Information File**. The results of this FE model are solely reported in Figure 2.9, as FEM Solid 3D, for the comparison study.

To evaluate the relative elastic modulus of an FE model, we consider two sides of the model perpendicular to FG direction x . An arbitrary displacement along x is applied to the nodes on one side, while the displacement of the nodes on the other side is fixed along x direction. In addition, for the 2D beam model, the rotation of nodes on the fixed side is set to zero. The equivalent stress is determined by dividing the resultant reaction force along the x direction at the fixed nodes by the apparent cross-sectional area of the model perpendicular to the load direction. Correspondingly, the equivalent strain is obtained by dividing the applied displacement by the length of the model along the x direction. Then, the effective modulus is computed by dividing the equivalent stress by the equivalent strain.

2.3 Method

2.3.1 Fabrication (3D printing) of honeycombs

The honeycombs specimens were fabricated using a Stratasys J750™ 3D printer, operating in high-quality mode with a layer height resolution of $27\mu\text{m}$ and a dimensional accuracy of $200\mu\text{m}$. All specimens were fabricated using Vero PureBlack™ material.

The mechanical properties of this material were determined through specific uniaxial tests following ASTM-D638 standards on the dog-bone samples shown in Figure B.9. During these auxiliary tests, a constant strain rate of 0.1 mm/sec was applied to the upper cross-head of the BETA 100 loading frame machine by MESSPHYSIK. The results yielded an average elastic modulus of $E_0 = 1436 \pm 10\text{ MPa}$. Additionally, the bulk material was estimated to have a density of $\rho_0 = 1.175\text{ g/cm}^3$.

The decision to use a printer that exploits material-jetting technology was made because it allows the production of almost isotropic samples with relatively small defects [10]. For each unit cell type, three different configurations were printed namely uniform, FG-regular, and FG-irregular, whose photographs are presented in Figure 2.5. For the uniform samples, the dimensionless thickness was considered to be $R = 0.25$ and the thickness was $t = 2 \pm 0.05\text{ mm}$. For FG samples, the degree of

graduation, (R_N/R_0) , measured as 2.88, 2.83, and 2.83 for HEX, TRI, and SQ samples, respectively, with a linear variation, i.e., $m=1$. The corresponding minimum thickness values were $t_0 = 1.35 \pm 0.05$ mm for HEX and SQ and $t_0 = 0.8 \pm .05$ mm for TRI unit cells.

The dimensions of all specimens are measured as 111 ± 0.5 mm $\times$ 88 ± 0.1 mm. To determine the relative density of the printed samples, accurate weight measurements were taken prior to the compression tests. The resulting relative densities from weight data have been documented in Table 2.1 and compared to those obtained from the CAD models and theoretically predicted by Equation (2.8). As seen in Table 2.1, the 3D-printed samples present slightly higher relative densities than both CAD and Equation (2.8).

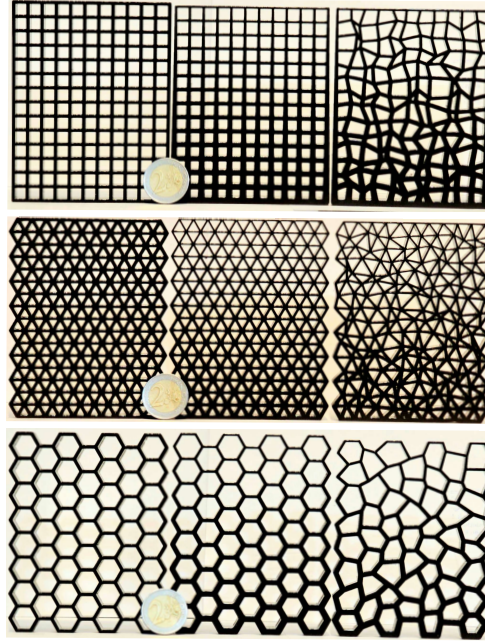


Figure 2.5. 3D-printed FG specimens for experimental tests. From top to bottom: lattice structures with SQ, TRI, and HEX unit cell, from left to right: uniform, FG regular, and FG irregular.

2.3.2 Compression test on 3D-printed honeycombs

In order to evaluate the accuracy of the refined Gibson-Ashby model for predicting the relative elastic modulus of the FG irregular honeycombs, a series of compression tests were conducted on the 3D-printed honeycombs. The honeycombs were tested under compression load by conducting a steady strain rate of 0.1 mm/sec to the

Table 2.1. The relative density ($\bar{\rho} / \rho_0$) computed by weighting the samples and comparing them with the corresponding CAD models and analytical expression in Equation (2.8).

		SQ	TRI	HEX
Equation (2.8)	Uniform	0.4471	0.6910	0.2742
	FG	0.5520	0.5879	0.3549
CAD Model	Uniform	0.4082	0.5722	0.2407
	FG-Regular	0.4897	0.4871	0.3078
	FG-Irregular	0.5042	0.4905	0.3158
3D-Printed	Uniform	$0.4830 \pm .0242$	$0.6791 \pm .0340$	$0.2863 \pm .0143$
	FG-Regular	0.5813 ± 0.0291	0.5812 ± 0.0291	0.3655 ± 0.0183
	FG-Irregular	0.5990 ± 0.0230	0.5841 ± 0.0292	0.3750 ± 0.0188

upper face of the specimens with a BETA 100 loading frame machine in order to assess the elastic modulus. Based on the ASTM-D638 guidelines, each configuration of the honeycombs was tested three times. Length changes were measured using a linear variable differential transformer arrangement between the platens to ensure accurate displacement measurement, accounting for frame compliance.

2.4 Results and discussion

This section compares the relative elastic modulus predicted by the proposed modified Gibson-Ashby model, FE numerical simulations, and results obtained from compression tests on the 3D-printed samples. The comparison demonstrates the applicability of the correction factors in capturing the effects of graded wall thickness variation and random irregularities. Firstly, all the fitting parameters in Equation (2.16) must be determined. The two parameters, C and n , from the standard form of the Gibson-Ashby equation, i.e., Equation (2.15), are calibrated to the uniform regular honeycombs. To determine these parameters, a range of uniform aspect ratios R_u is introduced into Equation (2.3) and Equation (2.4) to calculate the relative densities and corresponding relative elastic moduli. For HEX and SQ unit cells $0.05 \leq R_u \leq 0.5$ while for the TRI one, R_u is limited to 0.35 to avoid unrealistically high relative density values. By fitting Equation (2.15) to these pairs, values of the multiplier C and the exponent n are determined, as presented in Table 2.2. Note that Equation (2.4) is derived from structural analysis based on Timoshenko beam theory, meaning that the values of C and n are best fitted to this closed-form model.

Next, since the analytical relationship for determining the relative elastic modulus, Equation (2.4), is based on the assumption of a regular periodic geometry for the honeycombs, the FE model must be utilized to assess the effects of random irregularity and to calibrate the η correction factor. For this purpose, the degree of irregularity is incrementally increased by adjusting the Δ parameter within a range of 0 to 0.5, and

its impact on the equivalent elastic modulus of the honeycomb is evaluated via the FE simulations. Due to the random nature of irregularity, 20 random configurations (20 combinations of Λ_1 and Λ_2) are averaged for each value of Δ . The aspect ratio has been consistently maintained at $R_u = 0.25$ across all the models, i.e., $\kappa=1$, to isolate the effects of irregularity from the graded change in aspect ratio. Figure B.11 in **Supplementary Information File** plots the η values that fit the Equation (2.16) to the averaged FE results in a given Δ for all three honeycomb types. The results demonstrate that an increase in the Δ results in a dramatic decrease in the relative elastic modulus of honeycombs with SQ and TRI unit cells. For the extreme degree of irregularity with $\Delta=0.5$, the corresponding η values are 0.868 and 0.647, for TRI and SQ honeycombs, respectively, while the HEX unit cell shows almost no clear dependency on irregularity, offering $\eta=1$. It highlights the significant softening effect of random irregularity on TRI and SQ configurations. This is because introducing random irregularities in TRI and SQ lattices alters the deformation mechanism from stretching-dominated to bending-dominated, whereas the HEX design remains bending-dominated regardless of the irregularity. A best-fitting to the observed trend for the SQ and TRI configurations is performed. The fitting function, $\eta = f_2(\Delta)$, is presented in Table 2.2 for TRI and SQ irregular honeycombs.

In the subsequent step, the κ correction factor is fitted for FG honeycombs. To cover a broad spectrum of grading patterns, the dimensionless wall thickness ratio, (R_N/R_0) , is varied from 1 to 5, while the exponent m is set to 1, 2, and 3 to account for both linear and nonlinear variations. The effective relative density and effective relative elastic modulus are evaluated from Equation (2.8) and Equation (2.12). Substituting these effective values into Equation (2.16), and setting $\eta = 1$ to exclude irregularity, the correction factor κ is obtained across the range of $1 \leq (R_N/R_0) \leq 5$ for each exponent m . The calibrated κ values for HEX, TRI, and SQ lattices have been depicted in Figure B.10 in **Supplementary Information File**. In all cases, $\kappa=1$ when $(R_N/R_0)=1$, corresponding to uniform honeycombs, however, κ gradually decreases by increasing (R_N/R_0) . It means that the classical Gibson-Ashby equation fitted on uniform honeycombs overestimates the effective relative elastic modulus for FG ones. HEX honeycombs experience the highest softening due to the FG effect. A best-fitting for $\kappa = f(R_N/R_0)$ in the form of a quintic function, as presented in Table 2.2, is performed for each exponent m . The unknown coefficients are provided in Table B.1 in **Supplementary Information File**.

After calibrating the parameters, C , n , κ , and η , the ability of the modified model proposed in Equation (2.16) to reproduce trends in relative elastic modulus under varying grading and irregularity conditions is examined. Figure 2.6 displays the relationship between the relative elastic modulus and relative density for uniform honeycombs under both regular ($\Delta=0$) and high-degree irregularity ($\Delta=0.5$) conditions. FE simulations based on the Timoshenko beam element are provided for both cases. In addition, the analytical expression from Equation (2.5) and Equation (2.6) are presented solely for the regular honeycombs. To illustrate the modified Gibson-Ashby model in Equation (2.16), which assumes lattice uniformity ($R_0 = R_N = R_u$), the κ correction factor is set to 1 while the η correction factor varies depending on

Table 2.2. The calibrated parameters of the modified Gibson-Ashby model in Equation (2.16). The multiplier C and the exponent n are fitted to Equation (2.3) and Equation (2.4) for uniform honeycombs. The coefficients A_i for estimating the FG correction factor, k , are presented in Table B.1 in **Supplementary Information File** for $m=1, 2$, and 3, best fitted to Equation (2.8) and Equation (2.12). The random irregularity correction factor, η , is fitted to a set of randomly irregular FE simulations for different degrees of irregularity, Δ , as detailed in Figure B.11 in **Supplementary Information File**.

	C	n	$\kappa = f_1((R_N/R_0), m)$	$\eta = f_2(\Delta)$
HEX	0.66	2.43		1
TRI	0.53	1.37	$A_0 + \sum_{p=1}^5 A_P (R_N/R_0)^p$	$1 - 0.53\Delta^{2.01}$
SQ	0.69	1.21		$1 - 0.95\Delta^{1.43}$

the honeycomb type and the degree of irregularity, indicated by the Δ value. For the regular honeycombs, we set $\eta=1$. The results show an accurate agreement between the exact expression (hollow circles), and the modified Gibson-Ashby model (solid line), confirming the accuracy of the calibrated parameters C and n to the closed-form solutions in Equation (2.4). Moreover, the FE simulations for uniform structure (solid red circles) closely follow the modified Gibson-Ashby model (solid line) with a coefficient of determination, R^2 , equal to 1, 0.99, and 1 for HEX, TRI, and SQ regular honeycombs, respectively. It confirms the validity of the FE numerical approach. Additionally, for honeycombs with a high degree of irregularity, Equation (2.16) (dashed line) closely matches the FE results for irregular geometries (solid triangles) across the entire range of aspect ratios, confirming the accuracy of the calibrated η correction factor. The coefficient of determination, R^2 , is 0.95, 0.99, and 0.96 for HEX, TRI, and SQ irregular uniform honeycombs, respectively. Note that for HEX uniform lattice solid and dashed lines coincide, since $\eta=1$.

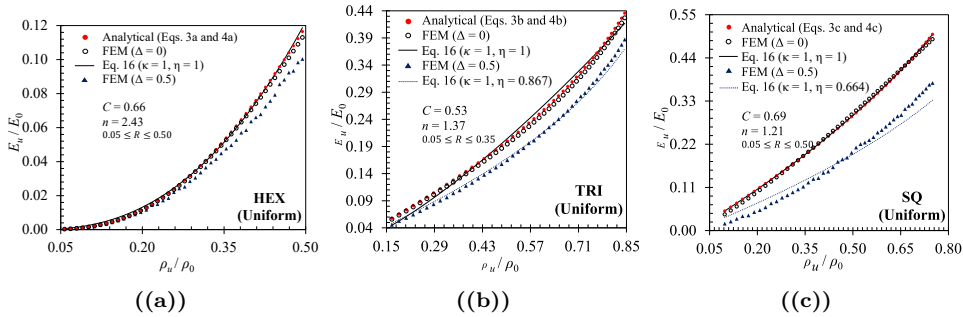


Figure 2.6. The comparison between the modified Gibson-Ashby model with FE simulations for the uniform regular ($\Delta = 0$) and irregular ($\Delta = 0.5$) honeycombs.

A remarkable accuracy for the calibrated multiplier C and exponent n is observed. The calibrated Gibson-Ashby model accurately fits the FE simulations for both regular and irregular uniform honeycombs.

Figure 2.7 illustrates the predicted values for the relative elastic modulus for regular and irregular ($\Delta=0.5$) FG honeycombs for the HEX, TRI, and SQ structures. The FE solutions are presented for both regular and irregular honeycombs, whereas the analytical solutions are provided only for the regular structures from Equation (2.8) and Equation (2.12). The classical Gibson-Ashby equation (Equation (2.15) without any correction factor), and the modified version with the κ correction factor suited to the FG type of honeycomb, detailed in Figure B.10 in **Supplementary Information File** are also plotted. The corresponding η correction factor is also applied to the irregular honeycomb configurations. Three different cases have been considered for reporting the results: a linear ($m = 1$) gradation with a moderate change in the dimensionless thickness ($R_N/R_0 = 3$), alongside an extreme variation in the dimensionless thickness ($R_N/R_0 = 5$) with linear ($m = 1$) and non-linear ($m = 3$) functionalities. In all cases, the values of R_0 and R_N are increased proportionally to maintain a constant ratio. For the lattice structures with HEX and SQ unit cells, the minimum and maximum values of the aspect ratio are set to 0.05 and 0.5, respectively, whereas, for the TRI honeycombs, the maximum aspect ratio is set to 0.35. For regular FG honeycombs, the modified model (solid lines) closely fits the analytical expression (hollow circles), confirming the accuracy of the calibrated κ correction factor. Besides, the FE simulations based on the Timoshenko beam element for regular lattices (solid red circles) accurately follow the modified Gibson-Ashby model (solid line) with a coefficient of determination, R^2 , equal to 0.99, 0.82, 0.99 for HEX, 0.97, 0.73, and 0.94 for TRI, and 1, 1, and 0.99 for SQ honeycombs for $(m, (R_N/R_0))$ pairs equal to (1, 3), (1, 5), and (3, 5), respectively. Comparing the modified model for irregular FG lattices with the FE simulations (solid triangles) illustrated an acceptable accuracy for the model. Although the κ and η correction factors are calibrated independently, the results demonstrate that the proposed modified equation with η correction factor effectively predicts the relative elastic modulus for irregular FG honeycombs across a broad spectrum of aspect ratio variations and high degrees of irregularity. The results obtained from the irregular FG lattice structure with the HEX unit cell align with those of the regular lattice structures, confirming the low sensitivity of the HEX honeycomb to the random irregularity.

Next, the accuracy of the localized (cell-by-cell) version of the Gibson-Ashby model introduced in Equation (2.18) is examined. For this purpose, both the relative density along the FG honeycomb, $\rho(x)/\rho_0$, and the corresponding relative stiffness values $E(x)/E_0$ are calculated directly from Equation (2.7) using the appropriate α parameter provided in Figure B.1 and Figure B.2 in **Supplementary Information File**. Subsequently, the $\rho(x)/\rho_0$ function from Equation (2.7) is inserted into Equation (2.18) and by incorporating the fitted values of C and n obtained from the curve-fitting on the corresponding uniform honeycomb, presented in Table 2.2, the value of $E(x)/E_0$ is predicted.

Figure 2.8 compares the predicted values of the relative elastic modulus using the exact analytical expression and the cell-wise application of the Gibson-Ashby model introduced in Equation (2.18). The local density values used along the FG direction correspond to the actual cell positions in the structure, with R_0 and R_N marking

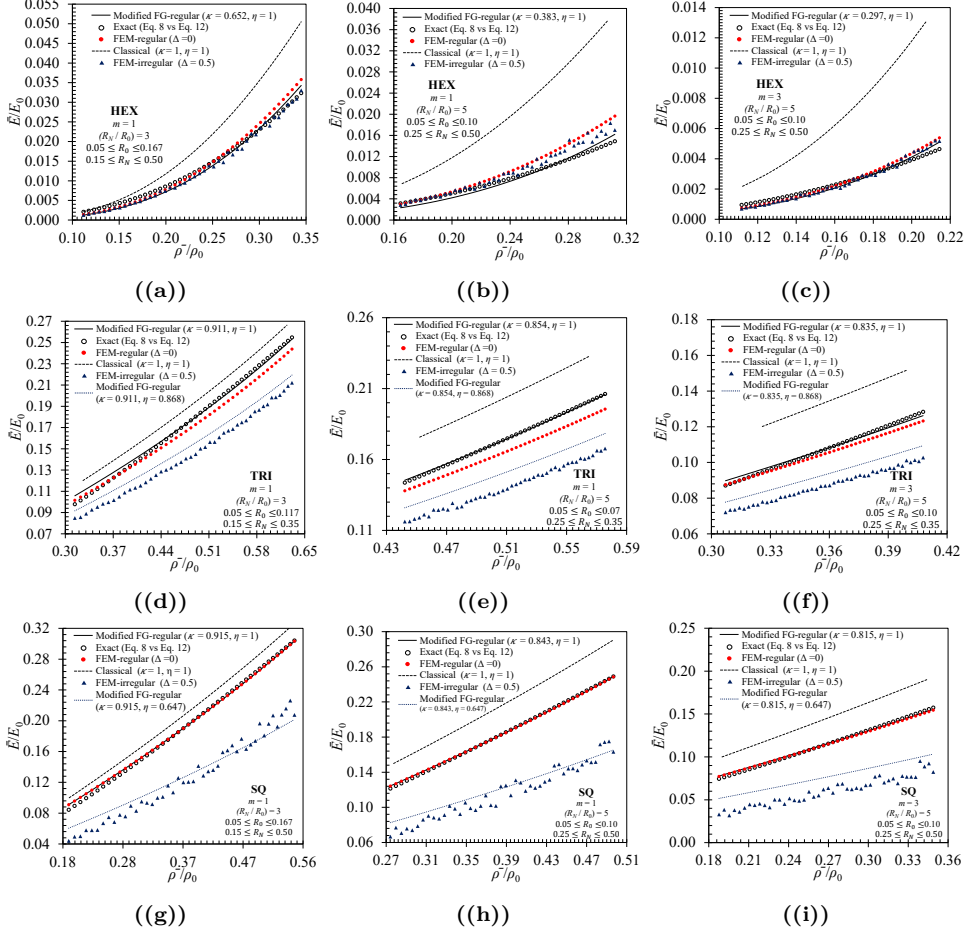


Figure 2.7. The Gibson-Ashby model for the uniform regular and irregular ($\Delta = 0.5$) honeycombs with a-c) HEX, d-f) TRI and g-i) SQ unit cell. The correction factors κ and η effectively fit the modified model to the FE simulations and analytical predictions. The classical Gibson-Ashby model is plotted to highlight its significant error in elastic modulus prediction for FG irregular honeycombs.

in the plots. The results confirm that this pointwise approach effectively captures the variation in elastic modulus with acceptable accuracy across the length of the functionally graded honeycomb.

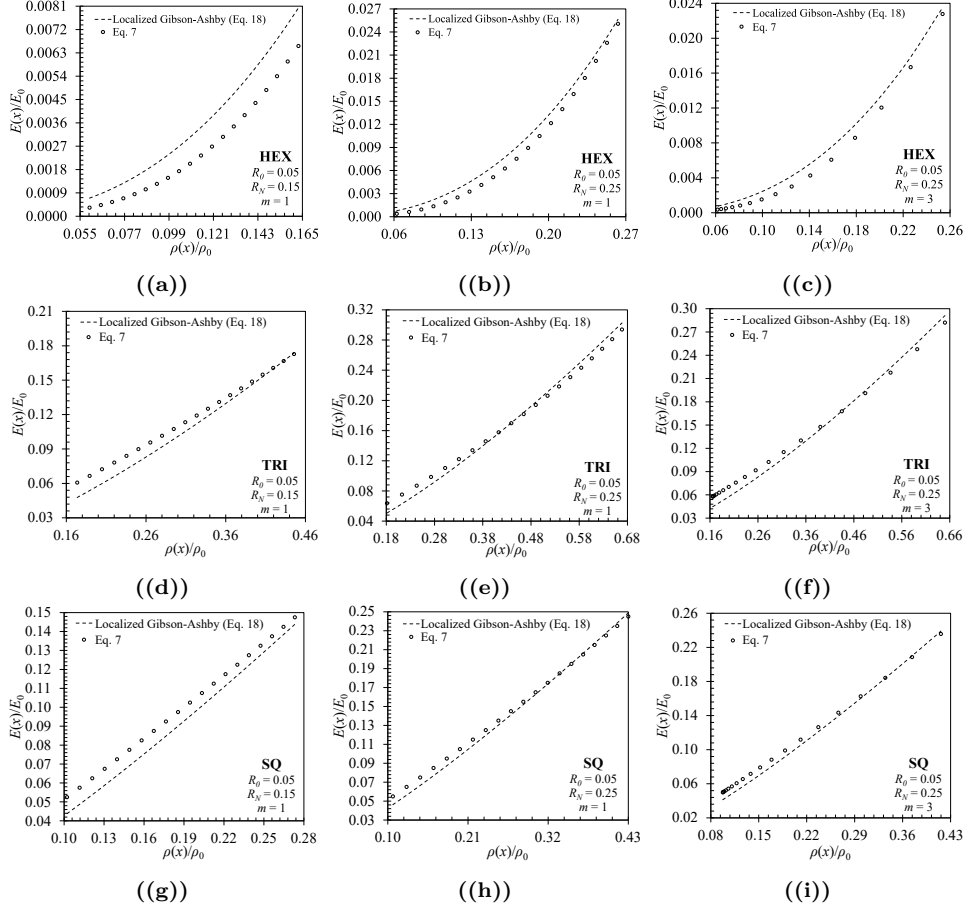


Figure 2.8. The local (cell by cell) Gibson-Ashby model. Comparison between the exact expression and the Gibson-Ashby models for honeycomb with a-c) HEX, d-f) TRI and g-i) SQ unit cell.

Finally, to assess the effectiveness of the correction factors κ and η , nine distinct samples were designed: three uniform, three FG regular, and three FG irregular structures with HEX, TRI, and SQ topologies. These samples were 3D-printed and underwent uniaxial compression tests to determine their relative elastic modulus, as presented in the Methods section. Additionally, the corresponding FE models for these nine designs were constructed based on the exact CAD model of the printed samples. Three different FE approaches were employed: a 3D solid model, a 2D plane-

stress solid model, and a Timoshenko beam model, resulting in 27 FE simulations in total. Details regarding meshing and boundary conditions are provided in the Methods section. For the given geometric parameters of the samples ($R_N/R_0 = 2.88, 2.83$, and 2.83 for the HEX, TRI, and SQ designs, respectively, and linear variation in all the samples, $m = 1$), the correction factor κ was found to be $0.67, 0.91$, and 0.92 from Table 2.2. Given the irregularity degree of 0.5 for all the samples, the corresponding values of η were determined as $1.00, 0.87$, and 0.66 from Table 2.2. Since these correction factors act as multipliers for the coefficient C in the Gibson-Ashby equation under a fixed exponent n , we first examined the ratio $C = (E_u/E_0)/(\rho_u/\rho_0)^n$ for the uniform structures. The experimental results from printed samples were compared with predictions from the three FE models (solid 3D, solid 2D plane-stress, and Timoshenko beam) in Figure 2.9 (a-c) for HEX, TRI, and SQ configurations. In the uniform case, both κ and η are unity, meaning that these plots directly represent the coefficient C , which establishes the relationship between relative modulus and relative density. The exponent n values are replaced from fitting to analytical expressions in Equation (2.3) and Equation (2.4) listed in Table 2.2, along with the relative densities from Table 2.1. As observed, there are discrepancies among the C values obtained through different methods, indicating that various modeling approaches yield different estimates for the relative modulus. As expected, the FE beam and solid models diverge when the length-to-cross-sectional ratio decreases. The discrepancy between the experimental and modeled results arises from multiple factors. First, as shown in Table 2.1, the theoretical predictions for relative densities by Equation (2.8) exhibit lower relative densities than printed specimens. Second, the Gibson-Ashby model, while effective for low-density cellular structures, becomes less accurate at higher relative densities (0.29 – 0.68 for 3D-printed samples), as widely documented in the literature. This limitation is inherent to the model itself. Third, the correction factors κ and η are fitted to a wide range of FG and irregular designs where a certain level of deviation in every fitting is unavoidable. Lastly, variability in the bulk material properties, particularly in 3D-printed polymers, contributes to deviations. The elastic modulus of the bulk material may differ when printed as a solid block in dogbone samples versus thin honeycomb walls due to differences in solidification conditions and defect formation. Thus, using the bulk elastic modulus from a printed solid reference sample as the denominator in relative modulus calculations introduces additional uncertainty.

Despite variations in C values for different methods in Figure 2.9 (a-c), it is essential to clarify that the goal of this study is not to tune C to fit the Gibson-Ashby model to experimental data. Instead, our objective is to assess whether the analytically derived κ and numerically determined η , based on Timoshenko beam simulations, can reliably capture the effects of FG and random irregularities in both experimental and solid FE models. To evaluate this, the corresponding correction factors were applied to experimental and numerical results in Figure 2.9 (d-i) for HEX, TRI, and SQ structures. The results demonstrate that introducing FG architectures and random irregularities consistently reduces the proportionality coefficient in the Gibson-Ashby equation, aligning with our model's predictions, where both κ and η

are less than unity. As expected, since these correction factors were calibrated based on Timoshenko beam theory, they accurately predict these effects in beam-based FE models with a maximum error of 6%. Notably, the same correction factors also provide reasonable predictions for 3D-printed samples, with a prediction error below 15%. Therefore, it is proved that the proposed correction framework serves as a practical tool for incorporating FG architectures and random irregularities in cases where the uniform Gibson–Ashby coefficient C is available. For denser honeycombs, where the standard Gibson–Ashby model tends to underestimate stiffness, the revised formulations by [53] offer improved predictions. While our study primarily focuses on the effect of functional grading and irregularities, incorporating their correction could further enhance accuracy in the high-density regime and will be considered in future work.

2.5 Conclusion

In this study, a modified model for predicting the elastic modulus of irregular FG honeycombs was developed by incorporating two correction factors into the classical Gibson–Ashby equation. These factors account for the gradual variation in wall thickness (κ) and random structural irregularities (η). Analytical approaches and FE simulations based on the Timoshenko beam theory were employed to determine these correction factors, and the accuracy of the model was validated against experimental tests on 3D-printed specimens. The results indicate that both functional grading and structural randomness lead to a reduction in the relative elastic modulus compared to uniform, periodic geometries, which are reflected in correction factors smaller than unity. More importantly, the proposed correction coefficients, although derived using the Timoshenko beam model, successfully captured the FG and irregularity effects in 3D-printed samples with a maximum error of 14.8% in experimentally measured relative elastic modulus of FG irregular samples. This highlights the effectiveness of the proposed correction framework in estimating the impact of randomness and FG variations in honeycombs by applying proper correction factors to a known uniform honeycomb modulus.

One of the key challenges in utilizing classical models such as Gibson–Ashby is their assumption of ideal, periodic structures, whereas real-world cellular materials often exhibit FG variations and irregularities. The proposed modified model bridges this gap by enabling rapid and accurate estimation of the elastic modulus without requiring extensive computational simulations or experimental testing. The proposed framework can be applied in optimizing honeycomb designs for engineering applications such as biomedical implants, impact absorption, and lightweight structures. For instance, in biomaterials, precise stiffness control in porous implants is crucial for improving mechanical compatibility with bone. Our model allows designers to estimate the effects of FG and irregularities on elastic modulus without expensive trial-and-error experiments. Although FE modeling is commonly used, this study provides

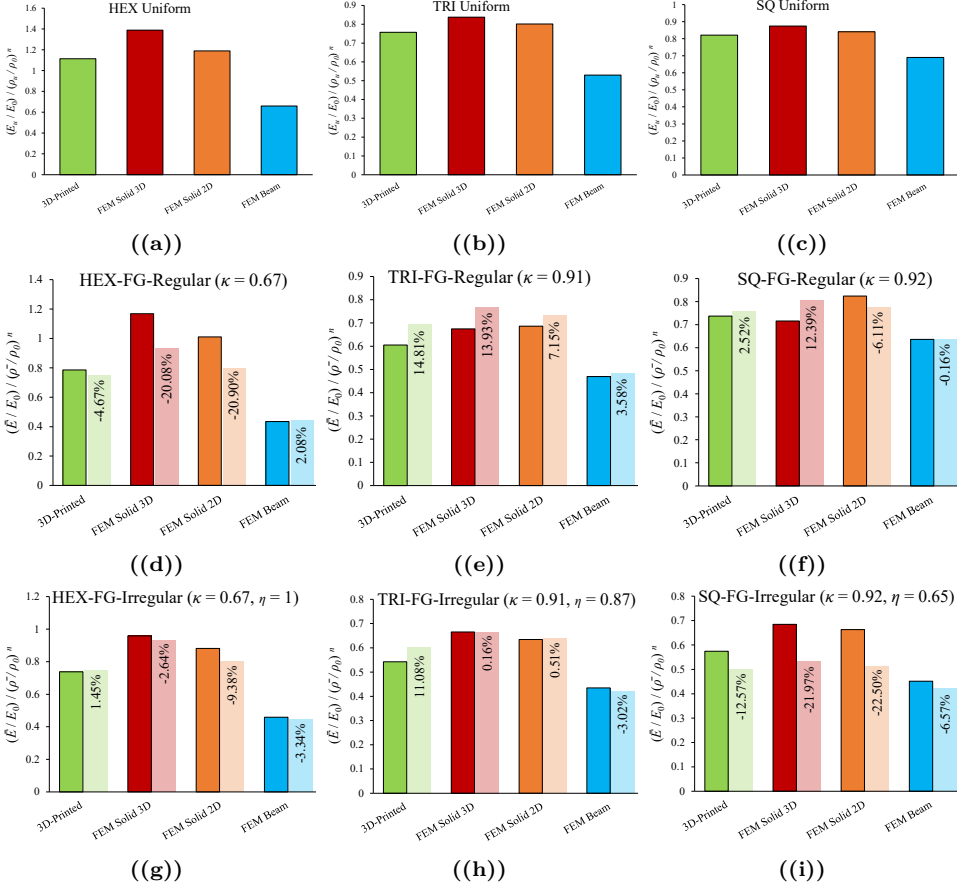


Figure 2.9. The validation study of correction factors in predicting the FG and irregularity effects on the relative elastic modulus of honeycombs. a-c) The multiple C values that fit the elastic modulus of 3D-printed and different FE simulations to the Gibson-Ashby model. d-f) The comparison study for the accuracy of the κ correction factor for FG-regular honeycombs. g-i) The comparison study for the accuracy of the η correction factor for FG-irregular honeycombs.

a systematic approach to evaluate the combined effects of functional grading and structural irregularities on stiffness, which is less explored in the current literature. Additionally, in aerospace and automotive industries, where lightweight yet robust structures are essential, this model offers a flexible and efficient framework for early-stage evaluation of mechanical performance in functionally graded cellular structures. Overall, this study provides a practical tool for estimating the elastic modulus of complex cellular materials.

CHAPTER 3

Adjusting Impact-Induced Wave Propagation in Elastic 2D Lattice Structures through Cell Geometry, Random Irregularity, and Mass Redistribution

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To be submitted in a Q1 high ranked journal

Abstract: This study explores how geometry-driven design strategies can tailor the dynamic response of two dimensional (2D) elastic lattices under transient impact loading. A total of 108 lattices based on 18 distinct unit-cell geometries are analyzed under equal global mass and wall length. Three geometric factors are examined: unit-cell topology, controlled irregularity introduced as random perturbations at wall junctions, and spatial wall-thickness grading (mass shifting). Finite element (FE) simulations show that unit-cell geometry dictates stress wave propagation trajectories. Controlled irregularity can further adjust wave propagation by promoting a switch from stretching- to bending-dominated deformation. A central contribution is the analytical modeling of graded lattices as a one-dimensional lumped mass-spring system employing the Gibson-Ashby model. A closed-form solution for a two-degree-of-freedom case provides physical insight into the effect of mass shifting. Results reveal that shifting mass toward the impact point reduces input acceleration and transmitted force, improving wave mitigation. The proposed model, while simple, captures these effects accurately and aligns well with FE results, offering a fast and reliable tool for designing mechanical metamaterials for stress wave attenuation.

Highlights:

- Wave propagation in 2D lattices is studied under transient impact loading.
- Random irregularities at junctions are shown to affect wave transmission.
- Graded wall thickness is used to shift mass distribution against the wave direction.
- A lumped mass-spring model captures the effect of graded mass and stiffness
- Wave speed, force transmission, and attenuation are tunable via geometry design.

keywords: Wave Propagation, Shock Mitigation, Impact Load, Functionally Graded Geometry, Random Irregularity, Metamaterials.

3.1 Introduction

Ongoing research in sustainable manufacturing, along with advancements in 3D and 4D printing technologies, continues to expand the capabilities of Additive Manufacturing (AM)-based engineered materials [1, 89]. These advanced technologies have facilitated the creation of lattice structures, functionally graded materials, and metamaterials, which are engineered to optimize the mechanical properties of materials by controlling their internal architectures [36, 90]. Cellular solids or lattices are structures configured by connecting a network of mechanical load-bearing components, such as struts, beams, or walls, that repeat spatially. These structures create a porous framework, that possesses unique mechanical properties, including a high strength-to-weight ratio and good energy absorption. Because of these features, they have attracted significant attention in aerospace, automotive, and other industries [91–94]. Among various types of cellular solids, or 2D lattice structures, also known as honeycombs, are of particular interest due to their simple geometry and ease of analysis. Honeycombs are typically created by extruding a 2D repeating unit cell along the third dimension. A key advantage of these structures is the ability to tailor their mechanical properties by modifying the unit cell geometry and its arrangement. The overall properties of the structure can be tuned by changing the unit cell geometry. A basic common unit cell shape is hexagonal, which has various geometric parameters that can be manipulated to achieve other unit cell shapes, such as rhombic, square, triangular, or auxetic unit cells with different mechanical properties [95]. Metamaterials, especially auxetic lattice structures, exhibit extraordinary mechanical behaviors not typically found in natural materials, most notably a negative Poisson’s ratio and tunable wave propagation characteristics. These unique properties make them highly attractive for advanced engineering applications such as vibration damping, impact mitigation, and acoustic insulation [42, 96]. The development of these innovative materials has been made possible by the precision and versatility of AM techniques, which enable the fabrication of complex geometries and customized material properties [38, 78].

Different analytical methods have been developed to investigate the mechanical properties of lattices based on the relative density [16, 18, 19]. Among analytical approaches, the Gibson-Ashby model is simple yet effective in predicting mechanical properties of 2D lattices [11]. However, due to the complexity of different unit cell geometries and various loading conditions, analytical methods are not always sufficient. Thus, many studies have turned to experimental and numerical methods to analyze these structures. Some research has focused on how the geometry of unit cells and their arrangements influence lattice behavior. Many studies have examined the mechanical properties of lattices under impact loading. Typically, numerical models simulate impact mitigation and energy absorption in lattices under high-impact forces

that cause complete and irreversible failure. These studies tune energy absorption by using different unit cell types and configurations [97]. For instance, functionally graded (FG) variations have been investigated in some papers [98]. [63,64,66,99]. Numerical simulations and experimental analyses highlight the impact of cell density and topological configuration on mechanical properties, with FG structures showing better support under small strain and enhanced energy absorption under large strain [36]. The gradation allows for optimized mechanical responses and substantial increases in energy absorption, making FG lattice structures a promising candidate for advanced engineering applications requiring high impact resistance and structural integrity. In addition to energy absorption, FG materials also play a crucial role in stress reduction by minimizing sharp material interfaces, which is particularly beneficial in applications such as prosthetic devices and high-temperature aerospace structures [100,101]. Dynamic analyses have shown that density grading can significantly enhance the energy absorption capabilities by altering the collapse mechanisms [62].

Beyond gradation, the introduction of irregularity in lattice structures offers another avenue for optimizing mechanical performance. Irregular lattice structures are particularly advantageous in applications where controlled deformation and impact mitigation are crucial, such as in aerospace crash protection [102,103]. The mechanical behavior of lattice structures under irregularity has been extensively studied, offering critical insights into their energy absorption, deformation mechanisms, and overall performance. Alkhader and Vural demonstrate that irregularity in lattice structures can shift deformation behavior from stretch-dominated to bending-dominated modes, which, while reducing stiffness due to increased bending moments and less efficient load sharing, offers a means to tune the balance between strength and toughness [80]. This is further supported by Chen et al., which investigates the constrained deformation of metallic foams, showing that irregular honeycombs more accurately capture size effects and strain distributions observed in experiments, outperforming regular models in representing real-world behavior [87]. Additionally, irregular lattice architectures have shown improved fatigue resistance and energy dissipation in cyclic loading conditions, making them highly suitable for vibration damping applications in the automotive and aerospace industries [104,105]. Montemayor et al. show that irregular structures exhibit higher stiffness but lower plastic-collapse strength compared to regular ones [81]. Collectively, these studies underscore that controlled irregularity can optimize energy absorption and impact resistance, offering a pathway for designing advanced cellular materials. However, designing and manufacturing these structures remains challenging due to the unpredictability of stress distribution and the difficulty of achieving precise control over irregularity. Recent advancements in stochastic modeling and AI-driven generative design have provided new avenues for optimizing irregular architectures while maintaining structural integrity [62,81].

A limited number of studies have examined impact wave propagation in elastic structures directly in the time domain, rather than the frequency domain. These studies focus on transmission of impact waves without destruction and have been done in one-, two-, and three-dimensions, focusing on wave propagation and force transmission at the structure's end [106,107]. Several works investigated wave propagation and

force transfer in single-component systems with variable geometry [108]. Building on these ideas, some researchers studied impact wave propagation in metamaterial structures. A regular hexagonal structure combined with a resonant beam-mass system was used to reduce impact effects [109]. The results showed up to 45% reduction in maximum output acceleration and 80% decrease in maximum support reaction. Some studies even took inspiration from nature. By mimicking DNA's double helix, a structure was designed where each unit cell acts as a double helical metamaterial [102]. Applying impact to this structure, input and output velocities and accelerations were measured. A reduction coefficient was defined as the ratio of the maximum output to the input acceleration to quantify impact mitigation. Results indicated that lattices with five unit cell repetitions could reduce impact effects by up to 65%. A similar study using lightweight chiral metamaterials also reported significant improvement in impact mitigation. They claimed up to a fivefold enhancement in reducing impact effects. Moreover, it was shown that increasing impact intensity led to greater reduction in impact effects [110].

Despite extensive research on lattice structures, time-domain studies on the propagation of mechanical impact waves in elastic 2D lattice structures remain limited. In this work, we investigate the influence of geometric variations, both at the unit cell level and in their arrangement, on the propagation of impact-induced waves in various lattice configurations. A total of 18 distinct lattice patterns, designed with comparable overall dimensions and mass, are initially developed. Irregularity is then introduced as an additional geometric parameter, followed by an FG variation in wall thickness to manipulate mass distribution against impact. Specifically, three mass distributions are considered by shifting material mass either toward or away from the impact location. This results in a comprehensive dataset of 108 lattice structures, calculated as $18 \times 2 \times 3$, where the factors correspond to lattice pattern, irregularity, and mass distribution, respectively. Dynamic finite element (FE) simulations in the time domain are conducted under impact loading conditions. To isolate and understand the individual effects of geometry, irregularity, and mass distribution, a normalization approach is adopted by introducing dimensionless correction factors. Key dynamic response parameters such as wave propagation speed, total energy, output acceleration sensed at the free end, input acceleration at the impact point, output-to-input acceleration ratio as the attenuation index, and transmitted force to the support are systematically analyzed. By comparing these metrics across the full design space, the study provides a detailed and quantitative understanding of how structural design choices influence impact wave propagation in elastic 2D lattices.

3.2 Problem Formulations

We consider a 2D lattice structure with an overall rectangular shape, defined in a global Cartesian coordinate system (x, y) whose origin is located at the bottom-left corner of the structure. Hereafter, *lattice* denotes a 2D lattice structure throughout

the text. The lattice has a total length L_x in the x -direction and a width L_y in the y -direction. The lattice is composed of a linear elastic, isotropic bulk material with density ρ_0 , Young's modulus E_0 , and Poisson's ratio ν_0 . The porosity parameter $\bar{p}$ (where $0 < \bar{p} < 1$) controls the amount of material removed from a fully solid volume to create the cellular geometry. Consequently, the total mass M and equivalent density $\bar{\rho}$ of the lattice are expressed as:

$$M = (1 - \bar{p})M_0, \quad \bar{\rho} = (1 - \bar{p})\rho_0, \quad (3.1)$$

where M_0 denotes the mass of a fully dense (non-porous) structure with the same external dimensions. A concentrated impact force $F(t)$ is applied in the negative x -direction at the midpoint of the right boundary, located at $(x, y) = (L_x, L_y/2)$. Two boundary conditions are considered. In the first scenario, the left edge at $x = 0$ is fully fixed, allowing for the analysis of support reactions and transmitted forces. In the second scenario, the left edge is free, and the resulting acceleration at its center, located at $(x, y) = (0, L_y/2)$, is analyzed to evaluate the dynamic response and momentum transmission. To enable meaningful comparisons across different lattice configurations under impact loading, all designs are normalized to have the same total mass and the same length along the impact direction, L_x . This ensures that the observed differences in structural response are attributable solely to variations in unit cell geometry and internal mass distribution, and not to size effects.

Three independent design variations are considered in this study. The first variation involves the choice of unit cell geometry, for which 18 distinct periodic regular designs are selected. The second variation introduces geometric randomness into these periodic structures, resulting in 18 corresponding irregular counterparts. The third variation involves shifting the mass distribution along the x -axis by gradually varying the wall thickness, implemented in two ways: a light-tip (LT) configuration, in which more mass is concentrated near the left edge ($x = 0$), and a heavy-tip (HT) configuration, in which the mass is shifted toward the impact end ($x = L_x$). This mass grading is applied to all 36 regular and irregular designs, yielding a total of 108 lattices, all with identical mass and length. The following subsections provide detailed formulations of these three design variations.

3.2.1 Unit Cell Geometry

The elementary building block of the studied lattices is a 2D unit cell defined in a local 1-2 coordinate system, as illustrated in Figure 3.1. The straight walls of length h are aligned with the 2-axis, while the inclined walls of length l form an angle θ with the 1-axis. The geometric aspect ratio defined as $\beta = \frac{h}{l}$. By fixing the inclined wall length l and varying h and θ , a variety of distinct lattice patterns can be generated from a unified parametric description. The regular hexagonal geometry corresponds to $\beta = 1$ and $\theta = \pi/6$, which serves as a reference configuration. In this configuration, the wall junctions are evenly distributed at six vertices forming a symmetric hexagon, as indicated by the black points in Figure 3.1. The number and positions of these

junctions vary with changes in β and θ , leading to different topologies. In the current study, five distinct lattice categories are defined based on specific combinations of β and θ :

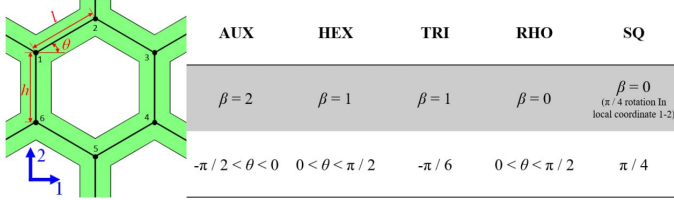


Figure 3.1. Geometrical parameter of the lattice unit cells.

- **Auxetic (AUX):** This category is defined by $\beta = 2$ and $\theta \in (-\pi/2, 0)$. These configurations exhibit negative Poisson's ratios and re-entrant angles, which are characteristic of auxetic behavior.
- **Hexagonal (HEX):** These patterns maintain a regular or stretched hexagonal geometry with $\beta = 1$ and $\theta \in (0, \pi/2)$. The internal angles remain acute, and the structure preserves its characteristic six-sided form.
- **Triangular (TRI):** When $\beta = 1$ and $\theta = -\pi/6$, the unit cell degenerates into a triangular configuration. In this case, two of the junction points (numbers 2 and 5 in Figure 3.1) coincide, resulting in the collapse of the hexagon and the formation of a triangle.
- **Rhombic (RHO):** Rhombic patterns are defined by $\beta = 0$, i.e., $h = 0$, meaning that the straight walls are eliminated entirely (coinciding junctions 1 with 6, and 3 with 4). The resulting geometry is formed solely by inclined walls, and θ can vary continuously within $(0, \pi/2)$ to control the internal angles of the rhombus.
- **Square (SQ):** This special case of the rhombic pattern occurs when $\theta = \pi/4$, yielding a square unit cell. To achieve alignment with the 1-2 coordinate system, the entire unit cell is rotated by $\pi/4$.

These five categories provide a representative set of structural motifs, enabling systematic investigation of how geometric parameters affect the mechanical and dynamic response of the resulting lattice materials, as depicted in Figure 3.2.

To construct the periodic regular lattices, the defined unit cells are tessellated in both global x - and y -directions to form planar lattices. Initially, an SQ unit cell, in which both the cell dimensions are equal to the inclined wall length l , is repeated uniformly. Specifically, the square unit cell is replicated $N_x = N_y = 11$ times, resulting in an overall lattice size of $L_x = L_y = 11l$. This square configuration is used as the reference pattern to match the global dimensions of the other lattice variants.

For all other unit cells, while maintaining a constant inclined wall length l , the number of repetitions in each direction is adjusted such that the total dimensions (L_x, L_y) of the generated lattice approximate those of the SQ configuration. Owing to the dependence of the unit cell size on geometric parameters θ and β , an exact match of the dimensions is generally not possible; however, the closest matching configuration is selected. For the HEX and AUX unit cells, which exhibit anisotropic properties, three inclination angles $\theta = \{0^\circ, 15^\circ, 30^\circ\}$ are considered. Given the anisotropic nature of these designs, each configuration is investigated under two orientations: one with the local 1-axis aligned with the impact direction (global x -axis), and the other with the local 2-axis aligned with the impact direction. This leads to $2 \times 3 = 6$ variants for each of the HEX and AUX patterns, yielding 12 lattice designs in total. For the RHO patterns, three values of $\theta = \{30^\circ, 45^\circ, 60^\circ\}$ are selected, resulting in three rhombic variants. The TRI configuration, which corresponds to a fixed angle of $\theta = -30^\circ$, is also analyzed under both local orientations, producing two additional cases. In total, this design framework results in 18 distinct lattice configurations. Figure 3.2 illustrates the layout of the periodic structures and their alignment relative to the impact direction. Table 3.1 presents the repetition counts (N_x, N_y) , total structure dimensions (L_x, L_y) , and unit cell length in the impact direction, l_c , for 18 lattice designs. A three-part coding system is used to identify each configuration, consisting of: (i) the structure type (AUX, HEX, TRI, RHO, SQ), (ii) the angle θ in degrees, and (iii) for anisotropic designs, the local axis (1 or 2) aligned with the impact direction. For example, the label AUX15(2) refers to an auxetic configuration with $\theta = 15^\circ$ where the local 2-axis is aligned with the impact direction, indicating that the straight walls are parallel to the applied load.

After defining the geometric layout of each unit cell and its repetition scheme, the final step involves assigning the wall thickness w_0 for each structure. The wall thickness is related to the porosity parameter, p , and governs the total mass of the lattice. To ensure a consistent mass across all 18 configurations, a numerical calibration was performed. For each configuration, the periodic lattice was constructed with the previously determined repetition numbers to approximate the reference size (L_x, L_y) . Then, through iterative adjustment, the wall thickness w_0 was tuned such that all structures shared the same total mass. The resulting values for wall thickness, w_0 , are summarized in Table 3.1. The 18 regular uniform (RU) lattices are shown in Figure C.1 in C.1.

3.2.2 Addition of random irregularity to regular lattice patterns

To investigate the influence of geometric imperfections, we introduced random irregularity into the 18 periodic lattice designs defined in Section 3.2.1, generating corresponding irregular (IR) structures. This method follows established approaches from the literature on lattice imperfection modeling [62,80,81,86–88]. Irregularity was introduced by perturbing the coordinates of the junction points that define the wall connectivity of each periodic lattice. Given the original position $(x_{\text{periodic}}, y_{\text{periodic}})$,

Table 3.1. Geometrical properties, mass, and porosity of the 2D lattice structures.

Pattern	θ	β	L_x [mm]	L_y [mm]	Nx	Ny	l_c [mm]	w_0 [mm]	Mass [g] (Porosity [%])			
									U		FG (HT or LT)	
									Regular	Irregular	Regular	Irregular
AUX30(1)	$\pi/6$	2	121.40	110.00	7	4	17.32	3.50	69.96 (48)	69.92 (48)	69.15 (48)	68.88 (48)
AUX30(2)			110.00	103.92	4	6	30.00	4.00	70.74 (38)	70.64 (38)	69.31 (39)	69.41 (39)
AUX15(1)			135.23	124.47	7	4	19.32	3.4	70.28 (58)	70.54 (58)	69.62 (59)	69.60 (59)
AUX15(2)			124.47	115.91	4	6	34.82	4.00	70.63 (51)	71.55 (50)	69.45 (52)	70.47 (51)
AUX0(1)	0	3	100.00	100.00	5	3	20.00	6.50	69.51 (30)	69.83 (30)	68.50 (32)	68.70 (31)
AUX0(2)			100.00	100.00	3	5	40.00	6.90	69.19 (31)	69.53 (30)	68.39 (32)	68.79 (31)
HEX30(1)	$\pi/6$	1	121.24	110.00	7	5	17.32	4.50	69.88 (48)	70.56 (47)	69.04 (48)	69.62 (48)
HEX30(2)			110.00	103.92	4	6	30.00	5.40	70.33 (38)	70.95 (38)	70.06 (39)	69.85 (39)
HEX15(1)			115.91	115.88	6	5	19.32	4.10	69.62 (48)	70.58 (47)	68.59 (49)	69.63 (48)
HEX15(2)			115.88	115.91	5	6	25.18	4.20	69.62 (48)	69.25 (48)	68.97 (49)	68.52 (49)
HEX0(1)	0	6	120.00	110.00	6	6	20.00	3.50	70.46 (47)	71.07 (46)	69.61 (47)	70.27 (47)
HEX0(2)			110.00	100.00	6	5	20.00	4.40	69.64 (37)	70.36 (36)	69.10 (37)	69.59 (37)
TRI30(1)	$-\pi/6$	1	121.24	110.00	7	11	17.32	1.80	70.31 (47)	70.80 (47)	69.34 (48)	69.70 (48)
TRI60(1)			110.00	103.92	11	6	10.00	2.00	69.18 (39)	69.81 (39)	68.11 (40)	68.54 (40)
RHO30(1)	$\pi/6$		110.00	103.92	11	6	10.00	3.00	70.78 (38)	71.47 (37)	69.53 (39)	70.18 (39)
RHO45	$\pi/4$	0	113.14	113.14	8	8	14.14	2.90	69.45 (46)	69.98 (45)	68.34 (47)	68.83 (46)
RHO60(1)	$\pi/3$		103.92	100.00	6	10	17.32	2.90	70.63 (32)	71.13 (32)	69.35 (33)	69.82 (33)
SQ	$\pi/4$	0	110.00	110.00	11	11	10.00	3.10	69.77 (42)	70.28 (42)	68.71 (43)	69.27 (43)
Average			114.02	108.39	7	6.30	20.67	3.89	70.00 (43)	70.46 (42)	69.07 (43)	69.43 (43)

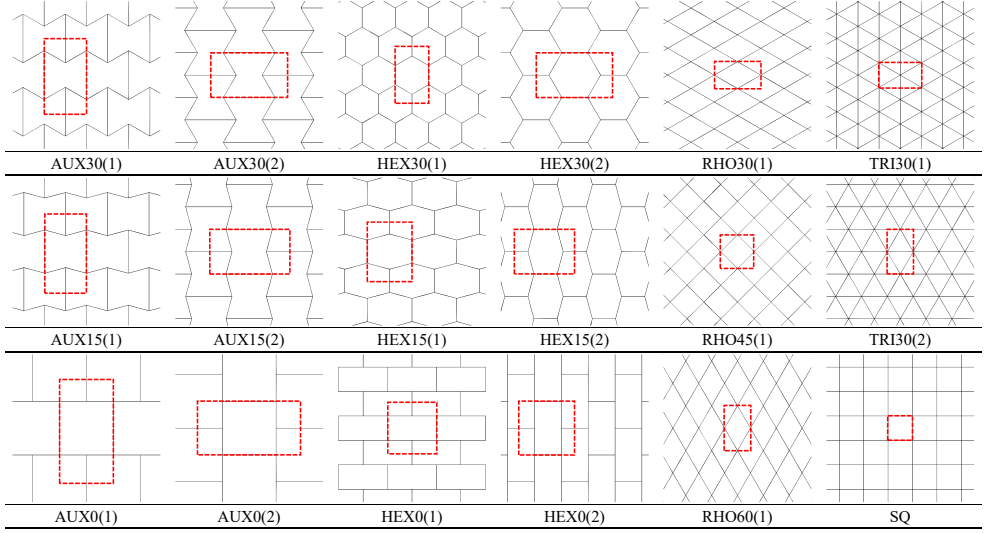


Figure 3.2. The 18 different 2D lattice patterns (the impact load direction is applied horizontally).

the new perturbed position $(x_{\text{irregular}}, y_{\text{irregular}})$ was calculated as:

$$\begin{aligned} x_{\text{irregular}} &= x_{\text{periodic}} + (\alpha_1 \Delta) \cos(2\pi\alpha_2)a, \\ y_{\text{irregular}} &= y_{\text{periodic}} + (\alpha_1 \Delta) \sin(2\pi\alpha_2)a, \end{aligned} \quad (3.2)$$

where $a = \min(h, l)$, defined as the smaller of the straight or inclined wall lengths, and Δ is a non-dimensional parameter controlling the magnitude of the irregularity. The variables α_1 and α_2 are independent random numbers in the range $[0, 1]$ for each junction. Geometrically, this approach relocates each junction to a random position within a circle of radius Δa centered at its original (periodic) location, as illustrated in Figure 3.3(a). The yellow markers indicate the unperturbed junctions, and the green circles define the allowable perturbation region for each. To prevent wall overlap, the value of Δ is constrained to $0 \leq \Delta < 0.5$. By applying this randomization procedure to all 18 periodic lattices, we generated 18 corresponding irregular (IR) configurations. These perturbed irregular lattices with uniform wall thickness (IRU) topologies are shown in Figure C.2 in C.1 for a non-dimensional parameter, $\Delta=0.25$.

3.2.3 Mass shift along impact direction

3.2.3.1 Wall thickness gradient along impact direction

To investigate the effect of mass distribution on impact response, we introduce a controlled wall-thickness gradient along the impact direction (x -axis) in the lattices.

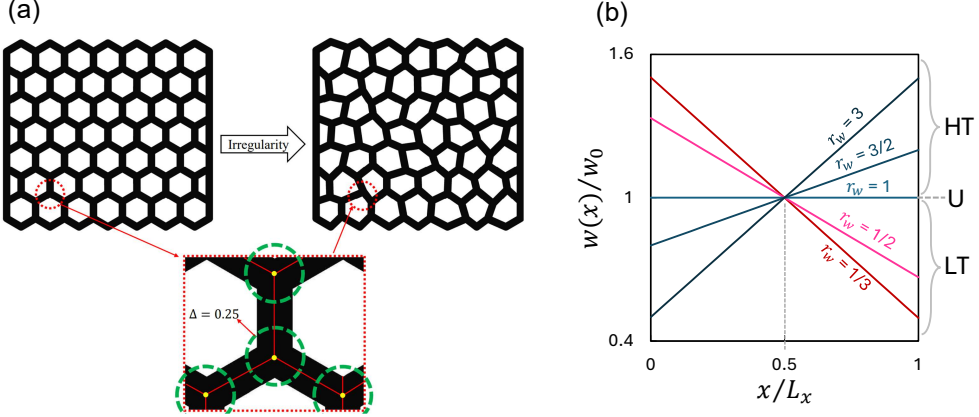


Figure 3.3. Modification scenarios for periodic lattices. (a) Schematic of applying a random irregularity to a HEX periodic lattice. (b) Variation of wall thickness across the lattice against impact load (x -direction) for different wall thickness grading parameters, r_w , resulting in heavy-tip (HT) and light-tip (LT) configurations.

By spatially varying the wall thickness $w(x)$ as a function of the coordinate x , the mass distribution is shifted toward or away from the impact edge. The thickness distribution is defined by the following expression:

$$\frac{w(x)}{w_0} = \frac{2}{1 + r_w} \left[(r_w - 1) \frac{x}{L_x} + 1 \right], \quad (3.3)$$

where w_0 is the baseline wall thickness corresponding to the uniform lattice (denoted by U), and r_w is a dimensionless parameter that controls the degree and direction of the thickness gradient. Indeed, by evaluating Equation (3.3) at $x = 0$ and $x = L_x$, it can be shown that $r_w = w(L_x)/w(0)$, representing the ratio of the wall thickness at the impact edge to that at the opposite edge. Equation (3.3) is formulated such that the wall thickness at the mid-point of the lattice ($x = L_x/2$) remains constant and equal to w_0 , ensuring direct comparability with the uniform configuration. The gradient is symmetric with respect to the center of the structure. Depending on the value of r_w , three distinct configurations are obtained. When $r_w = 1$, the thickness remains constant along x , i.e., $w(x) = w_0$, corresponding to the baseline uniform structure (U). When $r_w > 1$, the wall thickness increases toward the impact edge ($x = L_x$) and decreases toward the opposite edge ($x = 0$), effectively shifting the mass toward the loading side. This configuration is referred to as the heavy-tip (HT) design. Conversely, when $r_w < 1$, the wall thickness decreases toward the impact edge and increases toward the opposite edge, resulting in a light-tip (LT) configuration that reduces inertia near the loading side. As illustrated in Figure 3.3(b), this linear variation of wall thickness for different r_w values ensures a mass-neutral thickness variation, meaning that any increase in thickness on one side is balanced

by a corresponding decrease on the other, keeping the total mass constant across all configurations (U, HT, and LT), satisfying a fair comparison condition under equal-mass constraints. Applying HT ($r_w = 3$) and LT ($r_w = 1/3$) mass distributions to the 18 regular (Figure C.1) and 18 irregular (Figure C.2) lattices yields a total of 72 graded designs, whose geometries are illustrated in Figure C.3 to Figure C.5 in C.1. Combined with the 36 ungraded regular and irregular configurations, this results in 108 total lattice designs, each denoted by a five-part coding system. For example, AUX15(2)IRHT refers to an FG auxetic pattern with $\theta = 15^\circ$, whose 2-axis is aligned to the impact, modified by random irregularity (IR), and featuring a mass shift toward the impact side (HT configuration).

3.2.3.2 An equivalent 1D mass-spring system for graded lattice structure:

Here, we propose a simplified equivalent 1D mass-spring system for FG lattices with wall thickness gradients, that is, HT and LT designs. This model will be used later to interpret the effect of mass shifting against impact load on the time-domain response. For an FG lattice made of a bulk material with a density ρ_0 and Young's modulus E_0 , for a given percentage of porosity $\bar{p}$, the average density of the lattice, $\bar{\rho}$, is calculated from Equation (3.1). We assume that the density varies gradually and linearly along the impact loading direction in N discrete steps, from ρ_1 at the boundary end, which can be either fixed or free, and ρ_N at the impact location. The density in the i^{th} unit cell can thus be defined in terms of ρ_1 :

$$\rho_i = \left[1 + \frac{(i-1)(r_m-1)}{(N-1)} \right] \rho_1 \quad (3.4)$$

where $r_m = (\rho_N/\rho_1)$ is the degree of grading. When $r_m < 1$, the mass concentration shifts towards the boundary, resulting in an LT design, while for $r_m > 1$, the mass moves toward the tip, where the impact load is applied, i.e., HT design. $r_m = 1$ turns the lattice into a U design with a constant density equal to $\bar{\rho}$.

We establish a correlation between the lumped mass ratio, r_m , and the wall thickness ratio, r_w , defined as the ratio of the wall thickness at the tip to that at the boundary. The first lumped mass, m_1 , corresponds to the interval $x \in [0, \frac{L_x}{N}]$, while the last one, m_N , represents the interval $x \in [L_x(1 - \frac{1}{N}), L_x]$. Given the linear variation of wall thicknesses, the mass ratio r_m is defined based on the ratio of wall thicknesses evaluated at the center positions of these respective intervals, as illustrated in Figure 3.4(a). By substituting the center coordinates into Equation (3.3), the lumped mass ratio r_m is derived as a function of the wall thickness ratio r_w and the total number of masses N :

$$r_m = \left[\frac{(2N-1)r_w + 1}{2N + r_w - 1} \right]. \quad (3.5)$$

Figure 3.4(b) plots the ratio r_m/r_w as a function of N . As N increases, this ratio asymptotically approaches unity, since the center coordinates of the terminal masses converge toward the domain boundaries.

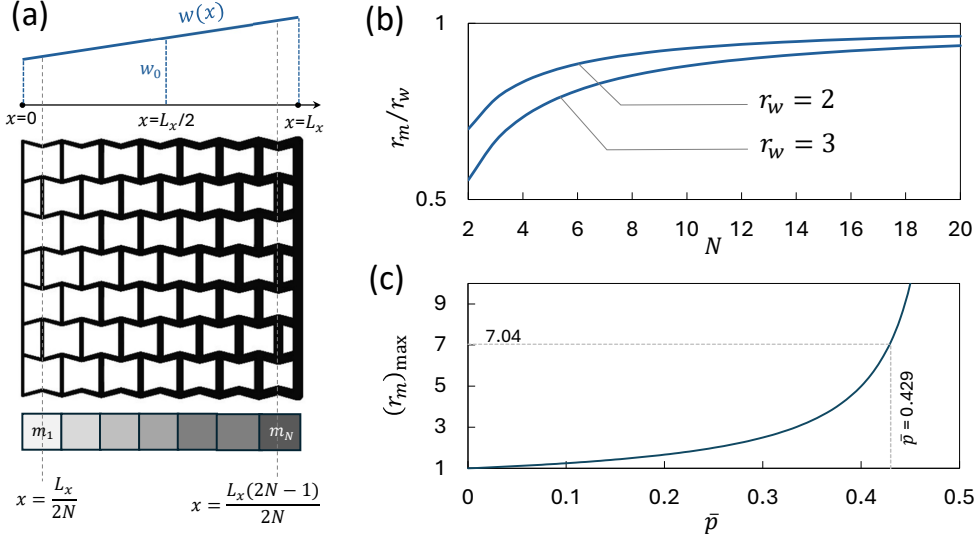


Figure 3.4. Mass equivalency between the lattice and the lumped mass system. (a) The center of the first mass, m_1 , and the last mass, M_N , are located at $x = L_x/(2N)$ and $x = L_x(1 - \frac{1}{2N})$. (b) The ratio of the wall thickness grading, r_w , to the lumped mass grading, $r_m = M_N/m_1$, as a function of N . (c) The maximum mass ratio, $(r_m)_{\max}$, as a function of average porosity, which is limited by the fact that the mass of cells cannot exceed the mass of a bulk cell.

For the total mass of the lattice to remain constant, the mean density across all unit cells must be equal to the average density:

$$\frac{1}{N} \sum_{i=1}^N \rho_i = \bar{\rho}. \quad (3.6)$$

Combining Equation (3.4) and Equation (3.6), the density of the i^{th} unit cell can be determined as:

$$\rho_i = G_i(1 - \bar{p})\rho_0, \quad (3.7)$$

where,

$$G_i(N, r_m) = \frac{1 + \frac{(i-1)(r_m-1)}{N-1}}{1 - \frac{r_m-1}{N-1} + \frac{(N+1)(r_m-1)}{2(N-1)}} \quad (3.8)$$

regulates the density distribution across the lattice with respect to the graded degree, r_m , while keeping the total mass constant. Provided that the density of cells cannot exceed the bulk density, Equation (3.7) implies that $G_i(1 - \bar{p}) \leq 1$. It yields an upper

limit for the mass ratio as,

$$(r_m)_{\max} = \frac{1}{1 - 2\bar{p}}, \quad (3.9)$$

which is plotted in Figure 3.4(c). After defining the stepwise density gradient by Equation (3.7), the Young's modulus in the i^{th} unit cell can be related to its density, ρ_i , by employing the Gibson-Ashby equation as,

$$\frac{E_i}{E_0} = C \left(\frac{\rho_i}{\rho_0} \right)^n, \quad (3.10)$$

where the multiplier C and the exponent n are the Gibson-Ashby model parameters, which can be determined analytically or by best-fitting experimental or simulation data for each lattice structure. It is analytically shown that for 2D lattices (honeycombs) the exponent n is 1 and 3 for stretch- and bending-dominated deformations, respectively [11]. Replacing ρ_i from Equation (3.7) into Equation (3.10), results in the stepwise grading function for Young's modules across FG lattices as,

$$E_i = C [G_i(1 - \bar{p})]^n E_0. \quad (3.11)$$

Multiplying both sides of Eq. Equation (3.7) by the unit cell volume, $A_c l_c$, gives the equivalent stepwise lumped mass grading along the impact loading direction as,

$$m_i = G_i(1 - \bar{p})m_0, \quad (3.12)$$

where $m_0 = \rho_0 A_c l_c$ is the mass of a unit cell fully filled by the bulk material. Similarly, the equivalent spring constant of the i^{th} unit cell can be obtained by multiplying both sides of Equation (3.11) by the ratio of cross-sectional area to unit cell length, A_c/l_c ,

$$k_i = C [G_i(1 - \bar{p})]^n k_0, \quad (3.13)$$

where $k_0 = (A_c/l_c)E_0$ is the spring constant of a unit cell fully filled by the bulk material. Given the stepwise grading functions for equivalent lumped mass and springs by Equation (3.12) and Equation (3.13), respectively, the FG lattice can be homogenized into a 1D lumped mass-spring system. This transformation reduces the system's degrees of freedom to N discrete points, denoted as x_1 to x_N . Figure 3.5(a) illustrates the equivalent mass-spring system representation of the FG honeycomb along with its corresponding degrees of freedom, and Figure 3.5(b) presents the simplest case, i.e., $N = 2$, with two degrees-of-freedom (2-DoF). The system of governing equations for this discrete equivalent model is defined in a matrix form as,

$$\begin{bmatrix} m_1 & 0 & \cdots & 0 \\ 0 & m_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & m_N \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \vdots \\ \ddot{x}_N \end{bmatrix} + \begin{bmatrix} k_1 + k_2 & -k_2 & \cdots & 0 \\ -k_2 & k_2 + k_3 & \cdots & 0 \\ \vdots & \vdots & \ddots & -k_N \\ 0 & 0 & -k_N & k_N \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ F(t) \end{bmatrix} \quad (3.14)$$

where, $\ddot{x}_i$ is the acceleration of the i^{th} lumped mass.

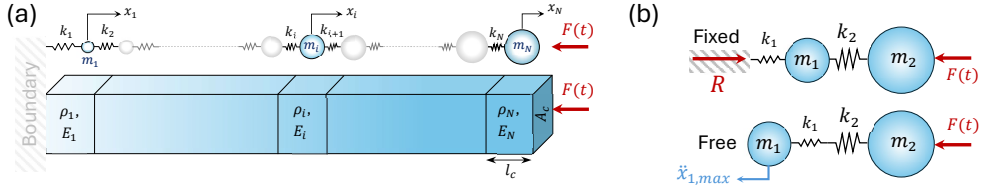


Figure 3.5. The schematic of the equivalent 1D mass-spring system. (a) Mimicking a lattice structure with a 1D mass-spring system consists of N lumped masses. (b) The simplest equivalent mass-spring system with $N = 2$ for free and fixed boundaries. Note that for the free end, spring k_1 is combined in series with spring k_1 .

3.3 Methods

3.3.1 FE analysis of lattice structures

Numerical simulations based on the FE method have been conducted to analyze the lattice structures under the impact load. A commercial software, COMSOL Multiphysics® has been used for the analyses. An isotropic linear elastic material with the Young's modulus $E_0 = 3.2$ MPa, $\nu_0 = 0.34$, and the density $\rho_0 = 1000\text{kg/m}^3$ is selected in our FE simulations. The geometries of 108 different lattices, presented in Table 3.1, are generated based on the procedure described in Section 3.2. The lattice walls have been modeled using the Timoshenko beam [111] in order to consider shear deformation. Each wall has been meshed with cubic and quadratic displacement and rotation fields, respectively. The number of mesh for each wall has been set to 10 for all the structures to ensure convergence in FE simulations [112].

Before dynamic analysis, a static study is conducted to examine the effective Young's modulus of the lattice configurations, which is used later in the interpretation of the results. For this purpose, a uniform displacement along x axis is applied to all the nodes on the right side, while all the nodes on the left side are fixed in the x direction, whereas other degrees of freedom are chosen free. The applied strain is calculated by dividing the applied displacement by the initial length of the lattice, L_x . The summation of the reaction forces in the x direction extracted from these nodes. The stress is calculated by dividing the total reaction force by the nominal cross-sectional area. The effective Young's modulus is then obtained by dividing the evaluated stress by the applied strain, as respectively illustrated for regular and irregular lattices in Figure 3.9(a) and (b) in Section 3.4.

For the dynamic analysis, a highly-transient impact load, shown in Figure 3.6, with time duration $\Delta t = 50$ ms and magnitude 4.4 N is applied to the middle of the right side at $(x = L_x$ and $y = L_y/2)$. A time step of $0.5\mu\text{s}$ is set for the transient solution. Two sets of boundary conditions (BC) have been taken into consideration: The fixed-free BC, where all the nodes on the left side are completely fixed, and the free-free BC, where the impact load is the only implemented boundary condition. Reaction

force is obtained from the fixed-free BC problem as the maximum magnitude of the time variant of resultant nodal forces in the x direction on the fixed side. Moreover, the wave speed is defined as $S = L_x/t_s$, where t_s is the traveling time of the incident wave to the fixed boundary. Furthermore, to calculate the attenuation index, which is defined as the ratio of the output acceleration sensed by the free end, a_o , to the imposed input acceleration at the point of applied load, a_i , we extract the maximum magnitude of acceleration of the nearest nodes to the middle points on the right and left sides. The schematic of the fixed-free and free-free BCs for time domain dynamic analysis is depicted in Figure 3.6.

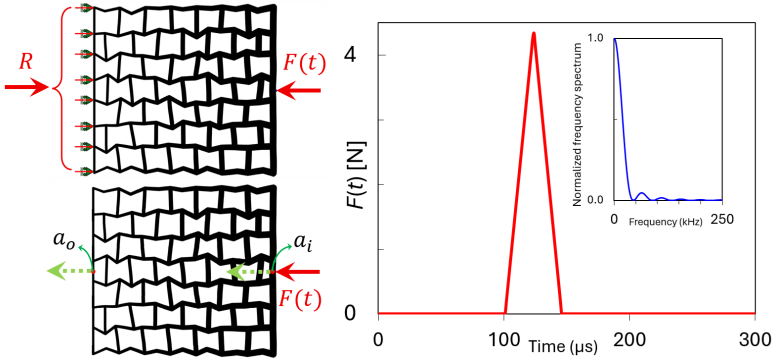


Figure 3.6. The schematic of the boundary condition applied to the time domain FE analysis.

3.3.2 Modal analysis of 2-DoF system under impact load

To offer an insight into the dynamic response of lattices under impact load, we analyze our proposed mass-spring model in Section 3.2.3.2 for the simplest case of 2-DoF setting $N=2$, whose schematic is represented in Figure 3.5(b). Generally, the equations of motion for a system with N degrees of freedom are a set of N coupled ordinary differential equations. These equations are difficult to analytically solve when the number of degrees of freedom is large or when the external forces are non-periodic. Modal analysis is a useful method to solve this problem. In this approach, the displacements of the masses are expressed as a combination of the system's normal modes, based on the expansion theorem, which makes it easier to find the closed-form solution. In the following, we explain the modal analysis procedure for a system with 2-DoF under impact load, whose equations of motion are simplified to:

$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \begin{Bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{Bmatrix} + \begin{bmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ F_2(t) \end{Bmatrix}, \quad (3.15)$$

where $F_2(t)$ is the external impact load which is applied on mass m_2 . Before applying modal method to solve above equation, it is necessary first to solve the eigenvalue

problem and find the natural frequencies ω_1, ω_2 and the corresponding normal modes $\vec{X}^{(1)}, \vec{X}^{(2)}$. The eigenvalue problem of Equation (3.15) is obtained as,

$$\left(\begin{bmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 \end{bmatrix} - \omega^2 \begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \right) \begin{Bmatrix} X_1 \\ X_2 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix}, \quad ([K] - \omega^2[M]) \vec{X} = 0, \quad (3.16)$$

which leads to:

$$\omega_1^2, \omega_2^2 = \frac{k_2(m_1 + m_2) + k_1 m_2 \pm \sqrt{[k_2(m_1 + m_2) + k_1 m_2]^2 - 4m_1 m_2 k_1 k_2}}{2m_1 m_2} \quad (3.17)$$

$$\vec{X}^{(1)} = \begin{Bmatrix} X_1^{(1)} \\ r_1 X_1^{(1)} \end{Bmatrix} = \begin{Bmatrix} 1 \\ r_1 \end{Bmatrix} X_1^{(1)}, \quad \vec{X}^{(2)} = \begin{Bmatrix} X_1^{(2)} \\ r_2 X_1^{(2)} \end{Bmatrix} = \begin{Bmatrix} 1 \\ r_2 \end{Bmatrix} X_1^{(2)}, \quad (3.18)$$

where r_1 and r_2 are,

$$r_1 = \frac{X_2^{(1)}}{X_1^{(1)}} = \frac{(k_1 + k_2) - \omega_1^2 m_1}{k_2} = \frac{k_2}{k_2 - \omega_1^2 m_2} \quad (3.19)$$

$$r_2 = \frac{X_2^{(2)}}{X_1^{(2)}} = \frac{(k_1 + k_2) - \omega_2^2 m_1}{k_2} = \frac{k_2}{k_2 - \omega_2^2 m_2}. \quad (3.20)$$

By orthogonalizing the normal modes with respect to the mass matrix, the values of $X_1^{(1)}$ and $X_1^{(2)}$ can be found as:

$$X_1^{(1)} = \sqrt{\frac{1}{m_1 + r_1^2 m_2}}, \quad X_1^{(2)} = \sqrt{\frac{1}{m_1 + r_2^2 m_2}}. \quad (3.21)$$

Based on the expansion theorem, the solution vector of the above equation can be expressed by a linear combination of normal modes:

$$\vec{x}(t) = q_1(t) \vec{X}^{(1)} + q_2(t) \vec{X}^{(2)}, \quad (3.22)$$

where $q_1(t)$ and $q_2(t)$ are time-dependent generalized coordinates. By defining a modal matrix as

$$[X] = [\vec{X}^{(1)} \quad \vec{X}^{(2)}] \quad (3.23)$$

Equation (3.22) can be rewritten as

$$\vec{x}(t) = [X] \vec{q}(t), \quad (3.24)$$

where

$$\vec{q}(t) = \begin{Bmatrix} q_1(t) \\ q_2(t) \end{Bmatrix}. \quad (3.25)$$

Using Equation (3.24), we can rewrite Equation (3.15) as

$$[M][X] \ddot{\vec{q}}(t) + [K][X] \vec{q}(t) = \vec{F}(t). \quad (3.26)$$

Premultiplying Equation (3.24) by $[X]^T$ yields

$$[X]^T [M] [X] \ddot{\vec{q}}(t) + [X]^T [K] [X] \vec{q}(t) = [X]^T \vec{F}(t). \quad (3.27)$$

By knowing $[X]^T [M] [X] = [I]$ and $[X]^T [K] [X] = \omega^2 [I]$, and defining $\vec{Q}(t) = [X]^T \vec{F}(t)$, Equation (3.27) can be simplified as

$$\ddot{\vec{q}}(t) + \omega^2 [I] \vec{q}(t) = \vec{Q}(t), \quad (3.28)$$

where

$$\vec{Q}(t) = \begin{Bmatrix} r_1 X_1^{(1)} F_2(t) \\ r_2 X_1^{(2)} F_2(t) \end{Bmatrix}. \quad (3.29)$$

Equation (3.28) denotes two uncoupled differential equations of second order:

$$\ddot{q}_i(t) + \omega_i^2 q_i(t) = Q_i(t), \quad i = 1, 2 \quad (3.30)$$

The solution of this equation can be obtained as

$$q_i(t) = \frac{1}{\omega_i} \int_0^t Q_i(\tau) \sin \omega_i(t - \tau) d\tau, \quad i = 1, 2. \quad (3.31)$$

By assuming the triangular shape for impact load according to Figure 3.6, $F_2(t)$ is defined as

$$F_2(t) = \begin{cases} 0, & t \leq t_0 \\ \frac{F_0}{t_1 - t_0}(t - t_0), & t_0 < t \leq t_1 \\ \frac{-F_0}{t_2 - t_1}(t - t_1) + F_0, & t_1 < t \leq t_2 \\ 0, & t > t_2 \end{cases} \quad (3.32)$$

and $q_1(t)$ and $q_2(t)$ are computed according to

$$\begin{aligned} q_1(t) &= \frac{r_1 X_1^{(1)}}{\omega_1} \left[\int_{t_0}^{t_1} F_2(\tau) \sin(\omega_1(t - \tau)) d\tau + \right. \\ &\quad \left. \int_{t_1}^{t_2} F_2(\tau) \sin(\omega_1(t - \tau)) d\tau \right], \quad i = 1, 2 \\ q_2(t) &= \frac{r_2 X_1^{(2)}}{\omega_2} \left[\int_{t_0}^{t_1} F_2(\tau) \sin(\omega_2(t - \tau)) d\tau + \right. \\ &\quad \left. \int_{t_1}^{t_2} F_2(\tau) \sin(\omega_2(t - \tau)) d\tau \right], \quad i = 1, 2 \end{aligned} \quad (3.33)$$

Substituting the triangular impact force from Equation (3.32) with $t_0=0$ and impulse duration of Δt , ($t_2 = \Delta t$, $t_1 = t_2/2$), into Equation (3.33) and integrating yields,

$$q_1(t) = \frac{2r_1 X_1^{(1)} F_0}{\omega_1^3 \Delta t} \left[3 \sin(\omega_1 t) + \sin(\omega_1(t - \Delta t)) - 2 \sin\left(\omega_1\left(t - \frac{\Delta t}{2}\right)\right) \right] \quad (3.34)$$

$$q_2(t) = \frac{2r_2 X_1^{(2)} F_0}{\omega_2^3 \Delta t} \left[3 \sin(\omega_2 t) + \sin(\omega_2(t - \Delta t)) - 2 \sin\left(\omega_2\left(t - \frac{\Delta t}{2}\right)\right) \right] \quad (3.35)$$

After finding the generalized displacements, $q_i(t)$, the physical displacement $x_i(t)$ can be found using Equation (3.24) as

$$\vec{x}(t) = \begin{Bmatrix} x_1(t) \\ x_2(t) \end{Bmatrix} = [X] \begin{Bmatrix} q_1(t) \\ q_2(t) \end{Bmatrix} = \begin{Bmatrix} X_1^{(1)} q_1(t) + X_1^{(2)} q_2(t) \\ r_1 X_1^{(1)} q_1(t) + r_2 X_1^{(2)} q_2(t) \end{Bmatrix}. \quad (3.36)$$

For considered 2-DoF system Figure 3.5(b), the support reaction is equal to the spring force k_1 and it can be calculated as

$$R = k_1 x_1(t) = k_1 (X_1^{(1)} q_1(t) + X_1^{(2)} q_2(t)) \quad (3.37)$$

For computing the attenuation index of the considered system, the spring connected to the support is relocated in the middle of the masses. It updates the k_1 and k_2 spring stiffnesses to zero and $(k_1 k_2)/(k_1 + k_2)$, respectively, and then the updated system of equations is solved to obtain the input and output accelerations.

3.4 Results and Discussion

This section presents the FE time-domain simulation results for lattices subjected to impact loading. The investigated response characteristics include the wave propagation speed (S), the total internal energy (W), the maximum transmitted force to the fixed BC (R), the input peak acceleration sensed at the impact point (a_i), the peak acceleration at the opposite side under free BC (a_o), and the attenuation index defined as $a_r = a_o/a_i$. The procedures used to extract these outputs from the simulations are described in Section 3.3. We select lattice configuration HEX30(1)RU as the reference for geometrical definition. For this structure, the baseline response vector is defined as:

$$\bar{P} = \{\bar{S}, \bar{W}, \bar{R}, \bar{a}_i, \bar{a}_o, \bar{a}_r\}. \quad (3.38)$$

Three independent strategies are considered for modifying the lattice design in order to tailor its response to impact: (i) altering the unit cell geometry, (ii) introducing random irregularities in the wall junctions, and (iii) redistributing the mass against the impact point while keeping the total mass constant. Each modification affects the response differently, and their influence is represented by three correction factors: C_g^P for unit cell geometric variation, C_Δ^P for random irregularities in wall junctions, and C_m^P for mass redistribution. The overall response of the modified lattice is expressed as a scaled version of the reference response by applying these correction factors:

$$P = C_g^P \cdot C_\Delta^P \cdot C_m^P \cdot \bar{P}, \quad (3.39)$$

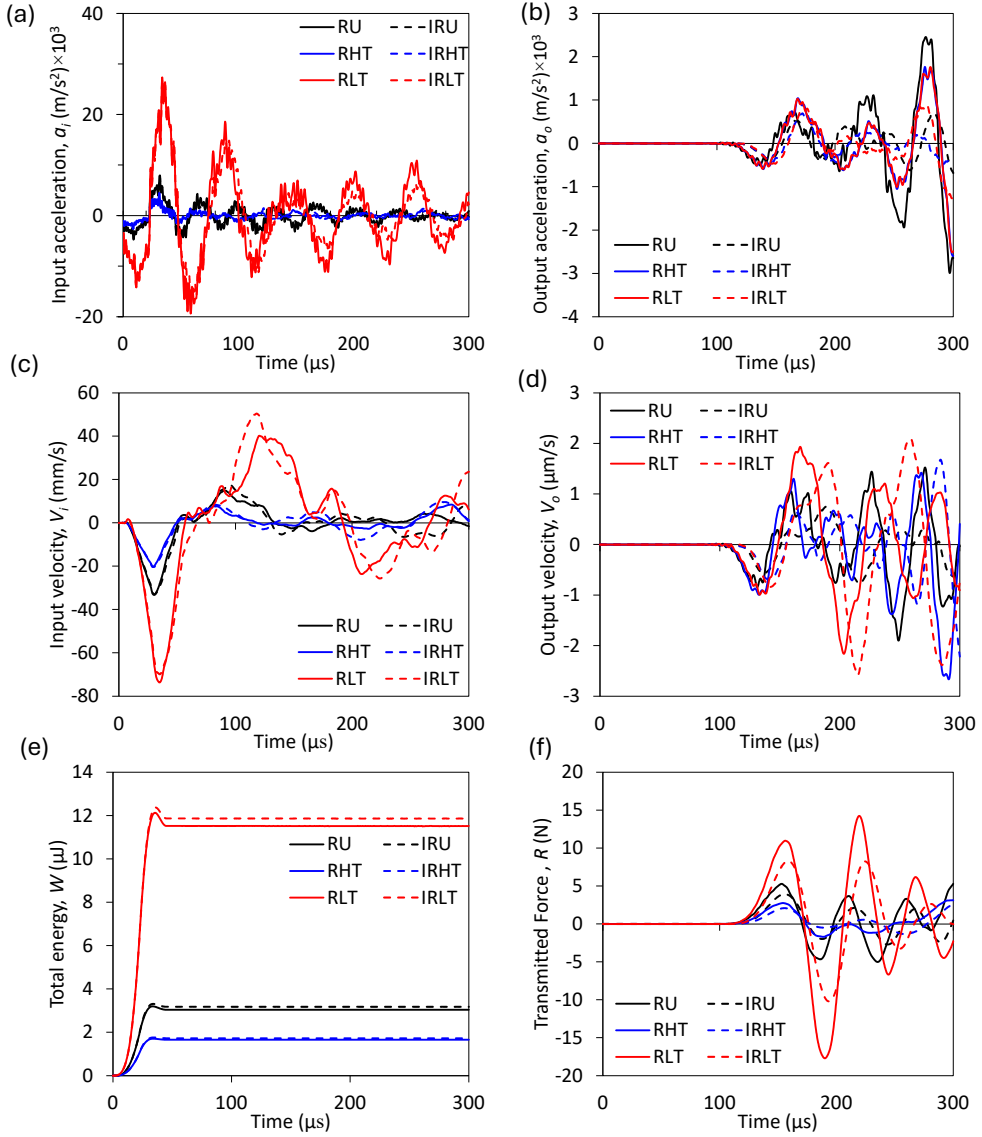


Figure 3.7. The time histories obtained from FE analysis for the reference lattice HEX30(1)RU, (a) input acceleration, (b) output acceleration, (c) input velocity, (d) output velocity, (e) total internal energy, (f) resultant reaction force at the fixed boundary nodes along impact load as the transmitted load to the support.

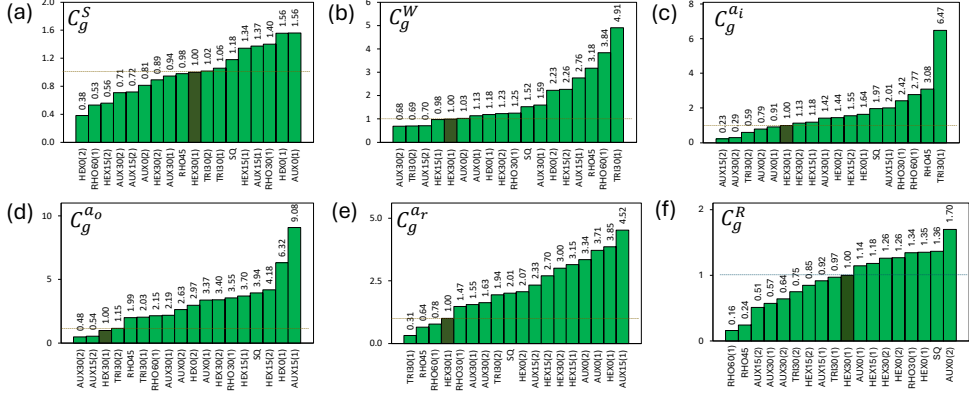
where $P = \{S, W, R, a_i, a_o, a_r\}$ denotes the impact response characteristics of the modified configuration. In the next three subsections, the influence of each modification strategy on the impact response is systematically evaluated using FE simulation results. For each of the 18 unit cell designs and all six response characteristics, the corresponding correction factors are presented. Furthermore, in the case of mass redistribution, additional insights are provided using an analytical modal analysis based on the equivalent 2-DoF mass-spring system, as described in Section 3.3.2, to explain the physical mechanisms governing the changes in response.

Due to the large number of designs and the volume of results, only the extracted key dynamic characteristics from FE time histories are presented to ensure clarity and avoid redundancy. However, as an example, the extraction procedure from the FE-generated time histories is detailed here for the reference configuration HEX30(1)RU. The same procedure is applied uniformly to all 108 lattices. Time histories of acceleration and velocity of incident and boundary nodes along the impact direction x , defined in Figure 3.6, the total internal energy, and the reaction force for the reference lattice structure, HEX30(1), are shown in Figure 3.7 (a) to (f), respectively. In this figure, RU, IRU, RLT, RHT, IRLT, and IRHT denote regular uniform, irregular uniform, regular light tip, regular heavy tip, irregular light tip, and irregular heavy tip lattices, respectively. From the time histories of accelerations from Figure 3.7 (a) and (b), the maximum magnitudes are extracted as a_i and a_o , respectively. Then, the attenuation index is calculated as the ratio of these maximum values, $a_r = a_o/a_i$. The wave speed, S , is obtained based on velocity tracking at the two assigned nodes along the impact direction, by dividing the distance between the two selected nodes to the time lags seen in Figure 3.7 (c) and (d). The plateaus observed in Figure 3.7(e) are defined as the total energy, W . In addition, the maximum magnitude of the time variant signals in Figure 3.7(f) for resultant reaction force along impact direction x is recorded as the transmitted force to the support, R . This procedure has been repeated for all 108 lattices, and the observations are discussed in the upcoming results.

3.4.1 Effect of unit cell geometry

In this section, the effect of unit-cell geometry on lattice dynamic response including the wave speed, the total internal energy, the input and output accelerations, the attenuation index, and transmitted force to the support is examined through the corresponding correction factors, i.e., $C_g^S, C_g^W, C_g^{a_i}, C_g^{a_o}, C_g^{a_r}, C_g^R$, respectively. To isolate the effect of cell geometry, neither random irregularities nor mass shifting is imposed. The 18 uniform lattices with various unit-cell geometries, as shown in Figure C.1 in C.1, have been considered, whose porosities and masses are detailed in Table 3.1 as U-Regular. Under impact loading and BCs described in Section 3.3, the dynamic responses are extracted from FE time histories. Then, setting $C_m^P=1$ and $C_\Delta^P=1$, the geometric correction factors, C_g^P , are obtained from Equation (3.39) as the ratio of the responses of each lattice to those of the reference lattice, HEX30(1)RU,

and are illustrated in Figure 3.8(a)-(f). Note that all the lattices have the same total mass and the same inclined wall length, l , resulting in different wall thicknesses, w_0 , as observed in Figure C.1 in C.1 and reported in Table 3.1.



concentrated impact load and lower local deformation, resulting in lower input acceleration and total energy. Nevertheless, the other three geometries, i.e., TRI30(1), RHO60(1), and RHO45, with the highest input acceleration and total energy, suffer from the lack of horizontal walls parallel to the load, particularly at the impacted point. It causes a dramatic growth in both input acceleration and total energy induced in the lattice. Figure 3.8(d) reveals that the acceleration at the opposite point (output acceleration) is tunable within ranges of 0.48 to 9.08. The lattice AUX15(1) has the highest, while AUX30(2) shows the lowest. The attenuation index for the

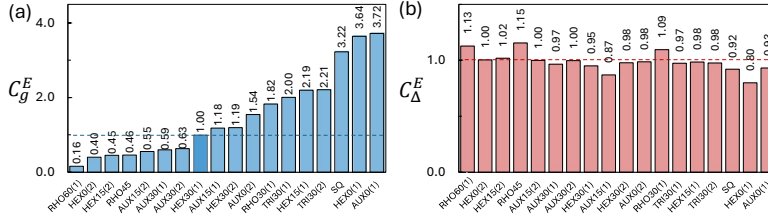


Figure 3.9. The effective Young's modulus of 18 different lattice geometries. (a) C_g^E that reflects the effect of unit cell geometry on the Young's modulus, defined as the ratio of Young's modulus to the reference lattice HEX30(1)RU. (b) C_{Δ}^E that presents the effect of random irregularity on the Young's modulus, defined as the ratio of Young's modulus of the irregular (IR) lattice to its regular (R) counterpart.

examined structures varies between 0.31 and 4.52 relative to the reference structure, with the TRI30(1) presenting the lowest and the AUX15(1) the highest ratio.

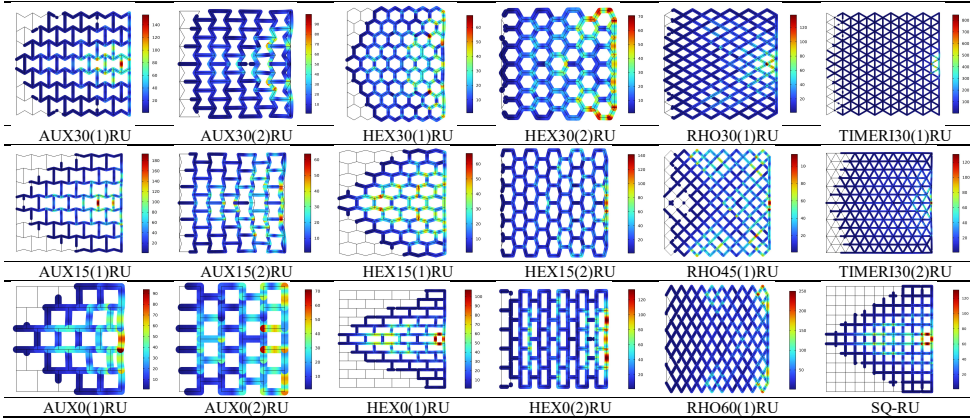


Figure 3.10. Stress wave propagation trajectories in 18 distinct regular lattice configurations with uniform mass distribution. The contour plots depict the moment when the stress wave is first detected at the fixed end, identified by the instant the von Mises stress exceeds a threshold of 1 kPa at the FE nodes on the fixed boundary.

As depicted in Figure 3.8(f), the magnitude of the transmitted force to the support

can be controlled between 0.16 to 1.7 times the reference lattice solely by altering the unit-cell geometry. Among the examined lattices, the RHO60(1) and the AUX0(2) lattices respectively lead to the lowest and highest transmitted load to the support. The configuration of the lattice, including the unit cell geometry and wall thickness, plays a significant role in the effective stiffness (see Figure 3.9(a)) and consequently in the time-dependent evolution of the dynamic response. In addition, the stress wave propagation trajectories through the lattices have a vital role, as illustrated in Figure 3.10. Notably, the RHO60(1) lattice, which exhibits the lowest effective Young's modulus among the examined configurations, results in the smallest support reaction force. The highest reaction force is observed in the AUX0(2) structure. Interestingly, although AUX0(2) does not possess the highest equivalent stiffness, it demonstrates a uniform wave propagation pattern across the lattice (see Figure 3.10). This uniformity facilitates near-simultaneous transmission of force to all support points, leading to a higher cumulative reaction force. It is a potential reason why the transmitted force for AUX0(2) surpasses the AUX0(1) lattice, although the latter has a higher effective Young's modulus. These observations underline the fact that, beyond effective stiffness characteristics, the global wave transmission behavior significantly influences how dynamic loads are distributed and resisted across the architected lattice structure.

3.4.2 Effect of random irregularity

In this section, the influence of applying random irregularity on the wall's junctions, as formulated in Section 3.2.2, is examined. The dimensionless perturbation parameter in Equation (2.14) is set to $\Delta = 0.25$. This irregularity generates 18 irregular uniform (IRU) lattice configurations from regular uniform (RU) counterparts with identical wall thickness. The geometries of these IRU samples are illustrated in Figure C.2 in C.1, while their porosities and masses, nearly identical to their regular counterparts, are summarized in Table 3.1 as U-Irregular. The reason for this mass consistency lies in the nature of the perturbation: although junctions are randomly shifted, the total wall length (and thus total mass) is negligibly affected.

Figure 3.11(a)–(f) illustrate the impact of the random irregularity on six key dynamic responses: wave propagation speed, total internal energy, input acceleration at the impact point, output acceleration at the opposite free BC, the attenuation index, and support reaction force under fixed BC. These are reported in terms of normalized irregularity coefficients, C_{Δ}^S , C_{Δ}^W , $C_{\Delta}^{a_i}$, $C_{\Delta}^{a_o}$, $C_{\Delta}^{a_r}$, and C_{Δ}^R , calculated according to Equation (3.39) as the ratio of the IRU lattice response to its RU counterpart. It is important to emphasize that these coefficients are evaluated independently from the geometry and the mass redistribution coefficients, setting $C_g^P=1$ and $C_m^P=1$ in Equation (3.39) for evaluating C_{Δ}^P coefficients.

As seen in Figure 3.11(a), for most lattice patterns, the wave propagation speed is only marginally affected by the irregularity. This is attributed to the fact that random irregularity alters the internal lattice geometry but leaves the global mass

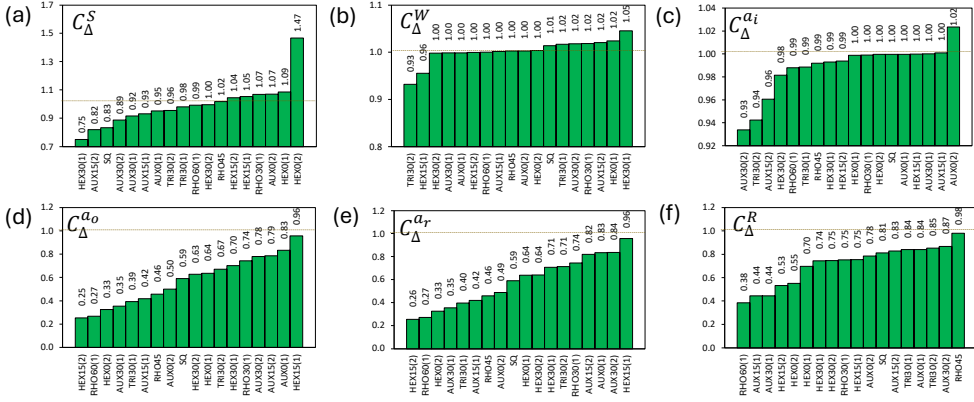


Figure 3.11. The correction factors, C^P_Δ , reflecting the effect of random irregularities for the dimensionless perturbation parameter, $\Delta = 0.25$. (a) The wave propagation speed, (b) the total internal energy, (c) the input acceleration, (d) the output acceleration, (e) the attenuation index, and (f) the transmitted load to the support.

distribution and density almost unchanged. It is consistent with the slight effect of irregularity on the effective Young's modulus of lattices compared to their regular counterparts, shown in Figure 3.9(b). Similar observations are made for the total internal energy and the input acceleration at the impact point in Figure 3.11(b) and (c), respectively, since irregularities do not modify wall thickness and mass at the impact side. However, as shown in Figure 3.11(f), the transmitted force to the support is generally reduced due to the presence of irregularity. The degree of reduction varies significantly across lattice unit cell types. For instance, the RHO60(1) structure shows a substantial reduction of up to 62%, while RHO45 shows only a minimal decrease of 2%. This discrepancy can be explained by the disturbance of the periodic alignment of the walls, which alters their orientation and participation in wave propagation. In some cases, this alteration may even shift the dominant deformation mode from stretching-dominated to bending-dominated behavior. In the case of the RHO60(1) lattice, the cell walls are predominantly misaligned with the impact direction, resulting in a strong bending-dominated load response. By contrast, the RHO30(1) lattice features walls that are more aligned with the impact direction, leading to a more stretching-dominated behavior. In both of these cases, the introduction of random geometric perturbations significantly alters the load-carrying mechanisms and the propagation of stress waves. On the other hand, the RHO45 structure, with its walls initially oriented at 45° relative to the impact direction, intermediate between RHO30(1) and RHO60(1), exhibits a more balanced response. Consequently, the presence of irregularity has a minimal effect on the overall mechanical behavior of this configuration. In the SQ configuration, two sets of walls exist: one aligned with the impact direction (maximally engaged) and one perpendicular (minimally engaged). Irregularity reduces the contribution of the former while increasing that of

the latter, resulting in a net reduction in reaction force, although not dramatically.

Similar to the transmitted force, the output acceleration at the free end generally decreases due to irregularity, as shown in Figure 3.11(d). Since the input acceleration remains nearly unchanged, this leads to a decrease in the attenuation index, defined as the ratio of output to input acceleration, depicted in Figure 3.11(e).

3.4.3 Effect of mass distribution shifting

This section investigates the influence of mass distribution shifting along the impact load direction on the dynamic response of lattices, through a set of the correction factors C_m^S , C_m^W , $C_m^{a_i}$, $C_m^{a_o}$, $C_m^{a_r}$, and C_m^R . Figure C.3 in C.1 illustrates a representative configuration of an FG lattice with a wall-thickness ratio of $rw = 3$ (and $rw = 1/3$ by rotating 180°), as defined in Equation (3.3). The correction factors are computed based on the ratio of dynamic response metrics between the regular FG lattice (with non-uniform wall thickness) and its corresponding RU lattice shown in Figure C.1 in C.1, using Equation (3.39), while the correction factors related to geometry and irregularity effects, namely C_g^P and C_Δ^P , are equal to unity. It thereby isolates the mass-shifting effect.

In addition to FE analysis, to assess the effect of mass redistribution, the FG lattices are approximated by an equivalent 2-DoF mass-spring model, formulated in Section 3.2.3.2, and analytically analyzed in Section 3.3.2. As presented in Table 3.1, the lattices exhibit an average porosity of $\bar{p} = 0.429$, an average length along the impact direction $L_x = 114$ mm, and an average transverse width $L_y = 108.4$ mm. A 2-DoF equivalent system yields $N = 2$, resulting in each equivalent unit cell having a length of $l_c = 114/2 = 57$ mm. An out-of-plane depth of 10 mm (identical to FE models) results in a cross-sectional area of $A_c = 1084$ mm² facing the impact load. The lattices are assumed to be made from a bulk material with density $\rho_0 = 1000$ kg/m³ and Young's modulus $E_0 = 3.2$ GPa, identical to the FE models. Three distinct mass distributions are considered along the impact direction: the HT configuration, where the wall thickness at the impact side is thicker than the opposite end ($r_m > 1$); the LT configuration with $r_m < 1$; and the U configuration with constant wall thickness along the entire length. Substituting the average porosity of $\bar{p}=0.429$ into Equation (3.9), yields the possible range for the lumped mass ratio parameter as $0.142 \leq r_m \leq 7.042$, see Figure 3.4(c). For each r_m within this range, the equivalent masses m_1 and m_2 are computed using Equation (3.12). The equivalent spring constants k_1 and k_2 are derived using Equation (3.13), under two idealized deformation assumptions: $n = 1$ for stretching-dominated behavior and $n = 3$ for bending-dominated behavior. The computed lumped masses and springs are subsequently substituted into the analytical solution to predict the impact response of the equivalent 2-DoF mass-spring system. In FE simulations, for 18 different FG lattices, four wall thickness ratios are assumed: $r_w = \{(1/4, 4), (1/3, 3), (2/5, 5/2), (1/2, 2)\}$. The first and the second in the parasyntesis correspond to LT and HT configurations, respectively. In order to compare to the equivalent mass-spring system, the

wall thickness ratios are converted to mass ratio via Equation (3.5) with $N = 2$, leading to $r_m = \{(0.54, 1.86), (0.60, 1.67), (0.65, 1.55), (0.71, 1.4)\}$.

Figure 3.12 illustrates the effect of mass distribution shift on three key dynamic response quantities: (a) the transmitted force to support, (b) the input acceleration at the impact point, and (c) the attenuation index, for the simplified 2-DoF lumped mass-spring system. These quantities are plotted as a function of the mass ratio r_m , and the best fits in the form of a power law, $C_m^P = r_m^\alpha$, are provided. The mass-spring predictions are compared with the corresponding FE simulations of the FG lattice structures. For each wall thickness ratio, the red solid circle is the average value of the 18 lattice patterns, and the red error bar is the standard deviation. In addition to averages and deviations, the individual responses of lattices are presented and compared for the case of $r_w = 1/3$ (LT, the red bar graphs) and $r_w = 3$ (HT, the blue bar graphs).

3.4.3.1 Mass shift toward the impact, HT configuration

As is evident in Figure 3.12, in the HT configuration, where the mass is shifted toward the impact location, both the transmitted force to the support and the input acceleration at the impact point decrease. The greater the shift (i.e., the higher the mass ratio r_m), the more significant the reduction in both responses. Conversely, the attenuation index increases with increasing mass concentration toward the impact point. The best-fit exponential scaling exponents for the transmitted force are found to be $\alpha = -0.5$ and $\alpha = -1.2$ for $n = 1$ and $n = 3$, respectively. For the input acceleration, the exponents are $\alpha = -1$ and $\alpha = -1.5$ for the same values of n . In contrast, the attenuation index grows linearly with the mass ratio for both $n = 1$ and $n = 3$, with $\alpha = 1$. Comparison with FE simulation results, shown as average values with standard deviation bands, indicates that for HT shifting, the simplified 2-DoF mass-spring model, despite its simplicity, effectively captures the mitigation effect of mass redistribution on the reaction force and impact-point acceleration, as well as the enhancement of the attenuation index. The blue data bars in the corresponding bar graphs represent individual lattice responses, specifically those with wall thickness grading $r_w = 3$, corresponding to the structures shown in Figure C.3 in C.1. Although the average trends align well with the mass-spring predictions, a wide variation exists among different lattice geometries. For example, the RHO45 lattice shows a 64% reduction in reaction force when mass is shifted to the impact end, whereas most other lattices exhibit a reduction in the range of 40–50%. HEX30(2) offers a slight mitigation as low as 6%.

For the input acceleration at the impact point, the 2-DoF mass-spring model predicts correction factors of $C_m^{a_i} = 0.60$ and 0.47 for $n=1$ and 3 , respectively, comparable to the mean FE result of 0.6 . Most of the investigated lattices fall within this range, with the exception of HEX30(2) and HEX0(2), which offer even a slight increase of 4% in the input acceleration due to mass shift toward the impact. For the attenuation index, the mass-spring model predicts a constant value of $C_m^{a_r} = r_m = 1.67$. This prediction closely matches the FE average of 1.65 . However, the attenuation in-

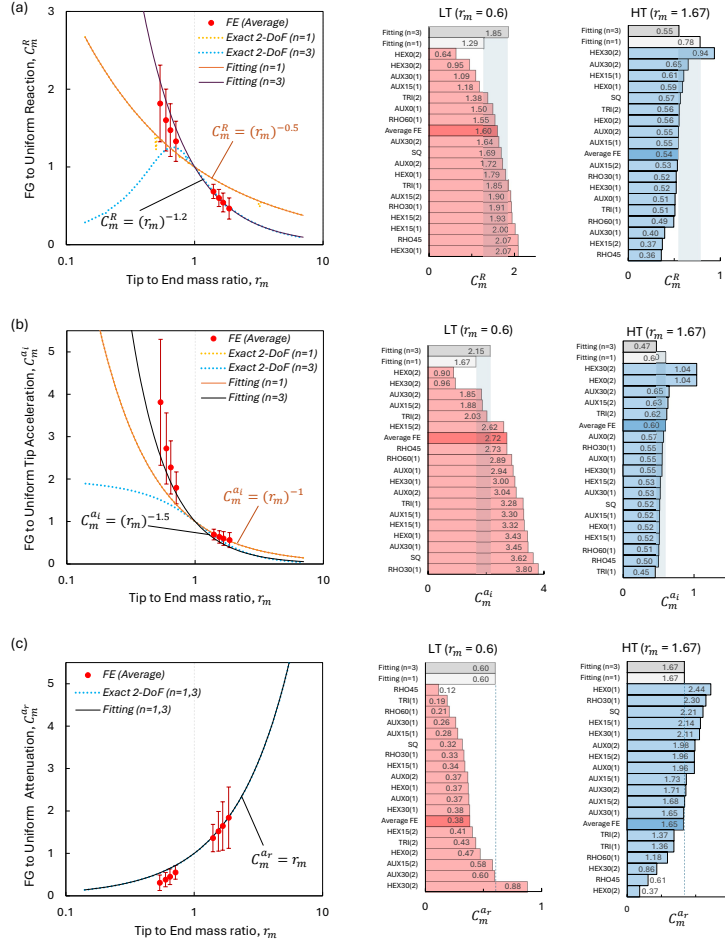


Figure 3.12. The Effect of mass distribution shifting on the dynamic characteristic response with respect to mass ratio, r_m in terms of C_m^R , $C_m^{a_i}$, and $C_m^{a_r}$ correction factors. The analytical predictions based on the modal analysis of the equivalent 2-DoF mass-spring system are presented (dotted lines) for stretching ($n = 1$) and bending ($n = 3$) dominant lattices. The power-law best-fittings (solid lines) are also provided in the form of $(r_m)^\alpha$. The averages (solid red circles) and standard deviations (the red error bars) of FE predictions for 18 different FG honeycombs are depicted for eight wall thickness ratios, $r_w = \{1/4, 1/3, 2/5, 1/2, 2, 5/2, 3, 4\}$. In order to compare, the wall thickness ratios are converted to mass ratio via Equation (3.5) with $N = 2$. (a) The transmitted force, (b) the input acceleration, and (c) the attenuation index. The bar graphs provide the details of the dynamic responses of all 18 lattice patterns for LT and HT mass distributions with $r_m = 0.6$ ($r_w = 1/3$) and $r_m = 1.67$ ($r_w = 3$), respectively.

dex across different lattice geometries spans a wide range. Notably, three structures, HEX0(2), RHO45, and HEX30(2), exhibit values of $C_m^{a_r} < 1$. This implies that, contrary to both the average trend and the mass-spring prediction, shifting mass toward the impact point actually reduces the attenuation index for these specific lattices. Meanwhile, other lattices show substantial enhancement, with some exceeding a 100% increase in the attenuation index due to mass concentration near the impact site.

3.4.3.2 Mass shift away from the impact, LT configuration

The shift of mass distribution away from the impact location, the LT configuration, is represented in Figure 3.12 by the left zone, where $r_m < 1$. The averaged values from the FE simulations indicate that both the transmitted force and the input acceleration at the point of impact increase as the mass is moved away from the impact site. This trend becomes more pronounced with a greater degree of mass shift in this direction. In contrast, the attenuation index remains primarily governed by the mass ratio r_m , showing a consistent decrease as r_m decreases (i.e., when the wall at the impacted side becomes thinner and the wall at the opposite side becomes thicker).

Regarding the transmitted force, the equivalent 2-DOF mass-spring system with $n = 1$, which corresponds to a linear variation in stiffness across the lattice length (same as the mass variation), accurately reproduces the trend observed in the FE simulations. It closely follows the power-law behavior fitted for the HT configuration, with the exponent of $\alpha = -0.5$. However, the mass-spring model with $n = 3$ predicts a non-monotonic response, with a peak in the transmitted force followed by a decline as the mass shifts further from the impact location. This nonlinearity is attributed to the significant softening (i.e., cubic decrease in stiffness) at the impact site due to mass depletion and reduced local density, which is representative of a bending-dominant regime in lattice structures. This non-monotonic trend is observed in the red bar plots of transmitted force in Figure 3.12(a), only for HEX0(2) and HEX30(2), with LT configuration showing lower transmitted forces than their U counterparts ($C_m^R < 1$). For the remaining lattices, and therefore for the overall average, the FE results follow the $n = 1$ model prediction, with the LT configuration consistently transmitting more load compared to the U configuration. Interestingly, when extending the fitted power-law relationship of the HT configuration (with $\alpha = -1.2$) to the LT range, as shown by the solid black line in Figure 3.12(a), the average FE results fall within the envelope defined by the two analytical models for $n = 1$ and $n = 3$. This implies that the equivalent mass-spring model, despite its simplicity, still offers a reasonably accurate prediction of the dynamic force response, even for the LT configuration where the mass at the impact site is significantly reduced.

A general trend similar to reaction force is observed for the input acceleration at the impact location, although the mass-spring system with $n = 3$ does not capture the clear peak followed by a decay in the mass-spring predictions across the LT range. Nevertheless, it fails to replicate the steep rise in input acceleration observed in the FE results for the LT lattices. Here again, the extension of the power-law fit from the

HT configuration (with $\alpha = -1.5$), depicted by the solid black line in Figure 3.12(b), provides a better prediction of the average lattice behavior in the LT domain. Once again, the HEX0(2) and HEX30(2) lattices behave differently from the rest: in the LT configuration, they show slightly lower input acceleration than the U case (10% and 4%, respectively), while in the HT configuration, their input accelerations are slightly higher (by 4%).

Finally, Figure 3.12(c) demonstrates that both the analytical solution and the averaged FE results provide consistent predictions for the attenuation index across the LT range, with both indicating a decline as mass is shifted further from the impact site. The mass-spring model predicts a strictly linear decreasing relation with respect to r_m , similar to the HT case, with an exponent of $\alpha = 1$. However, the average FE values suggest a sharper-than-linear decrease. This is evident from the red bar graph for LT with $r_m = 0.6$ for individual lattices, where FE predictions of $C_m^{a_r}$ for all lattices (except HEX30(2)) are lower than the mass-spring model prediction of 0.6.

In summary, the analytical model by the equivalent 2-DoF mass-spring system, developed based on the Gibson–Ashby model for the effective modulus of lattice, provides a satisfactory approximation of the dynamic response of the lattices, despite its simplifying assumptions. Its accuracy is particularly higher for the HT configuration, where the system inertia is concentrated toward the impact. Furthermore, both the FE simulations and the analytical model confirm that mass shifting along the impact direction can be effectively utilized as a design strategy for tailoring the dynamic response of architected materials.

3.4.4 Effect of combined mass distribution shifting and irregularities

In this section, we examine the combined effect of introducing random irregularity and mass shifting on the dynamic response of the lattices. To this end, the dynamic responses of the irregular lattices shown in Figure C.4 for IRHT and Figure C.5 for IRLT configurations are compared with their corresponding uniform regular counterparts in Figure C.1 in C.1. Since each irregular FG lattice is individually compared with its RU counterpart, the geometry correction coefficient C_g^P in Equation (3.39) equals unity. Moreover, because both irregularity and mass shifting are applied simultaneously, a combined correction coefficient $C_{m\Delta}^P$ is introduced to replace the individual correction terms C_m^P and C_Δ^P . Figure 3.13 presents the combined correction coefficients $C_{m\Delta}^S$, $C_{m\Delta}^W$, $C_{m\Delta}^{a_i}$, $C_{m\Delta}^{a_o}$, $C_{m\Delta}^{a_r}$, and $C_{m\Delta}^R$, corresponding respectively to wave speed, total energy, input acceleration, output acceleration, attenuation index, and reaction force at the support, for the 18 investigated lattices under both HT (light blue bars) and LT (light red bars) configurations. To assess whether the superposition of their individual effects can approximate the combined effect of irregularity and mass shifting, we compare the product $C_m^P \times C_\Delta^P$, obtained from Section 3.4.2 and Section 3.4.3 for each lattice, with the combined correction factor $C_{m\Delta}^P$. In Figure 3.13, the light surrounding thick bars represent the combined correction factors,

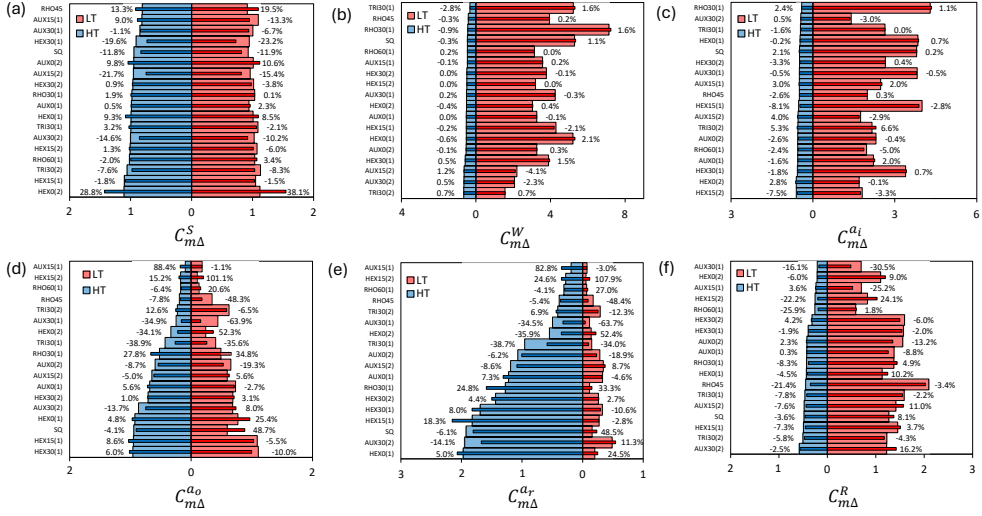


Figure 3.13. The combined correction factors for simultaneous application of random irregularity and mass shifting C_m^P (light surrounding thick bars). These combined factors are compared to the product of the individual correction factors, $C_m^P \times C_\Delta^P$ (dark central thin bars). The deviations (percentage) of the product compared to the combined correction factors are presented. Results reveal an acceptable accuracy of superposition for estimating the combined effect.

while the dark central thin bars indicate the product $C_m^P \times C_\Delta^P$ (blue and red for HT and LT, respectively). The deviations of the product of individual correction factors compared to the combined ones are also presented in percentage for each lattice design. The following average deviations are obtained for each dynamic response as, $10.1 \pm 8.8\%$ for wave propagation speed, $1.0 \pm 0.5\%$ for total energy, $1.8 \pm 2.8\%$ for input acceleration at the impact site, $27.5 \pm 18.0\%$ for output acceleration at the free end, $28.8 \pm 18.7\%$ for the attenuation index, and $10.3 \pm 7.4\%$ for the transmitted force to the fixed support. Overall, these results indicate that the superposition principle provides a reasonably accurate prediction of the combined effect of irregularity and mass shift on the dynamic response of the lattices. However, the accuracy is not uniform across all unit cell geometries, and in some cases, the deviation is more pronounced. The assumption of superposition shows excellent agreement for total energy and input acceleration, and good accuracy for the reaction force and wave speed. Nonetheless, the deviation is higher for the output acceleration under free-end BC, and consequently for the attenuation index. Despite these larger errors, the overall trend of the combined effect is still well captured by the superposition model. This observation suggests that, in both experimental and numerical studies, the combined effect of geometric irregularity and mass shifting in FG lattices can be reasonably approximated by independently evaluating their individual contributions.

As a result, the overall dynamic response can be reliably predicted without the need for additional combined tests or simulations, thereby reducing the experimental and computational effort.

3.5 Conclusion

This study provides a comprehensive investigation into the tailoring of impact-induced wave propagation in 2D elastic lattice structures through controlled variations in three key design parameters: unit cell geometry, topological irregularity, and mass distribution shifting. A large set of lattice designs was analyzed using time-domain FE simulations under impulsive loading, enabling a systematic evaluation of how these parameters, individually and in combination, affect critical dynamic response metrics, including wave speed, total energy, transmitted force, input, and output acceleration, and attenuation index. The main findings and contributions can be summarized as follows:

- **Unit Cell Geometry as a Primary Design Lever:** The geometry of the repeating unit cell plays a critical role in shaping the impact-induced dynamic behavior of lattice structures, even when the total mass and wall length are held constant. Variations in wall orientation with respect to the loading direction, the dominant local deformation mode (bending versus stretching), and the local arrangement of walls near the impact point strongly affect the initial input acceleration and the total energy transmitted into the structure. These geometric factors collectively influence the stress wave propagation paths, thereby modulating the force transmitted to the fixed boundary and the attenuation index at the free end. Remarkably, a substantial degree of tunability in all key dynamic metrics can be achieved solely through the selection of the unit cell geometry.
- **Geometrical Irregularity as a Secondary Tuning Parameter:** Introducing controlled irregularity at wall junctions through random perturbations emerged as an effective, albeit geometry-dependent, strategy for tuning dynamic responses. While a fixed level of irregularity was applied across different lattice topologies, the resulting effects varied significantly depending on the underlying cell geometry. Overall, the introduction of irregularity tends to attenuate the dynamic response, including reductions in transmitted force and attenuation index. This effect is particularly pronounced when the imposed irregularity switches the deformation mechanism between stretching- and bending-dominated behavior.
- **Mass Shift Modeling and Its Role in Tailoring Impact Response:** A central innovation of this study lies in the analytical modeling of the mass-shift effect along the impact direction in FG lattice structures. To capture the effect of gradually varying wall thicknesses, we developed an equivalent 1D discrete

mass-spring model. In this formulation, the gradual variation in wall thickness was first systematically related to spatial changes in density and mass distribution, which in turn were mapped onto changes in the lumped mass values in the discrete model. Using the Gibson–Ashby relation, density variations were further translated into a spatially graded Young’s modulus, allowing us to define a corresponding stiffness gradient for the springs. This enabled the construction of a reduced-order, physics-informed, and analytically tractable model capturing the essential behavior of FG lattices under transient impact loading. To assess the fidelity and predictive capacity of this approach, a modal analytical solution was derived for the simplest 2-DOF system under impulsive loads. Despite its apparent simplicity, this model exhibited strong agreement with full time-domain FE simulations, validating its ability to capture key trends in dynamic response induced by mass shifts. Our results demonstrate that shifting mass toward the point of impact leads to a reduction in the local input acceleration at the point of applied impact load and a significant decrease in the total input energy, which in turn reduces the transmitted force to the fixed boundary. Conversely, a mass distribution skewed away from the impact location results in higher input energy and stronger transmitted forces. However, in systems with free-end boundaries, the attenuation index, defined as the ratio of acceleration at the free end to that at the point of impact, decreases/increases when mass is shifted away from/toward the impact site. This behavior stems from the diminished input acceleration at the impact point. This insight emphasizes that mass-shifting is a tool to tune the wave propagation characteristics and dynamic transmissibility of elastic lattices under impact. Altogether, the mass-shift modeling framework introduced here offers a physically grounded, analytically tractable, and numerically validated method for engineering the impulse response of lattice materials. It not only provides a deeper understanding of how FG architectures control wave dynamics, but also provides an approach for designing optimized lattices with tailored impact mitigation.

- **Superposition-Based Design Implication:** A key outcome of this study is the validation of the superposition principle for predicting the combined effects of irregularity and mass shifting. While some discrepancies exist for specific cases, the overall trend and response behavior can be reasonably predicted by independently analyzing and combining individual effects. This enables substantial reductions in experimental and computational efforts for future design studies.

In conclusion, this research provides fundamental insights into the dynamic behavior of architected 2D lattice materials and introduces a flexible framework for tailoring their impact responses through multi-parameter structural design. The findings lay the groundwork for the development of advanced, application-specific metamaterials with optimized impact mitigation and stress wave manipulation.

Part II

Machine learning and multiple objective optimization

CHAPTER 4

Physically based machine learning for the multi-objective optimal design of partially recycled materials: The case study of rubber resources in the automotive industry

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Journal: Journal of Cleaner Production

Revised, Under review

Abstract: This study introduces a versatile framework that combines advanced artificial intelligence and multi-objective optimization with a mathematical model to accelerate the integration of recycled materials into virgin resources, addressing critical challenges in sustainable material management. Focusing on recycled rubber from End-of-Life Tires as a case study, we optimize the recovery of properties while balancing economic and regulatory constraints. The proposed framework combines a transparent and adaptable semi-analytical micromechanical model with a physics-informed optimization algorithm, enabling the simultaneous management of multiple additive strategies to minimize deviations from virgin material performance. By providing strategies for selecting and tailoring additives to recover diverse material properties, the model enhances decision-making processes. Validated through experimental calibration, our approach bridges the gap between recycling processes and practical applications. While demonstrated in the automotive industry, this scalable framework offers a generalizable solution for incorporating recycled materials into production processes, advancing circular economy practices and driving sustainable manufacturing.

Highlights:

- Wave propagation in 2D lattices is studied under transient impact loading.
- Random irregularities at junctions are shown to affect wave transmission.
- Graded wall thickness is used to shift mass distribution against the wave direction.
- A lumped mass-spring model captures the effect of graded mass and stiffness

- Wave speed, force transmission, and attenuation are tunable via geometry design.

keywords: Recycling, Waste Management, Micromechanics, End-of-Life Tires (ELTs), Machine Learning, Multi-Objective Optimization, Automotive Industry

4.1 Introduction

Recycling waste materials is essential for promoting sustainability and environmental protection. The European Commission’s “4R” framework—Reduce, Reuse, Recycle, and Recover—aims to optimize resource use and to minimize environmental harm by reintegrating recycled materials into production cycles, fostering a sustainable economic model [113,114]. Ideally, recycling aims to *recover the lost properties* of primary raw materials during their transformation into products, allowing them to be reused in the same primary applications. Optimizing the recycling process is critical to producing high-quality recycled materials that can replace (even partially) virgin resources, balancing performance, cost, and regulatory requirements [115,116]. However, it demands a multi-objective optimization approach to ensure recycled materials meet necessary criteria while remaining cost-effective [117]. These optimal recycling processes support sustainable manufacturing, expand the adoption of recycled materials across various industries, and contribute to resource efficiency and environmental conservation by reducing waste disposal impacts [118–121].

Given the rapid growth of artificial intelligence techniques, their role as efficient tools for developing and optimizing recycling process models has become increasingly indispensable. For an efficient recycling process, establishing a versatile framework for mathematically modeling the recovery properties of recycled materials is essential. Then, this framework can be integrated seamlessly with machine learning models and support multi-objective optimization algorithms to identify optimal recycling strategies. This study aims to introduce a simple, efficient, and accessible model to achieve this. Although its adaptability allows it to be calibrated for diverse recycling optimization scenarios across various sectors, as a demonstration, we applied the proposed framework to address the global challenge of tire recycling in the automotive industry.

The increasing number of vehicles has led to a growing demand for tires, and once tires become unsafe for use, they are classified as end-of-life tires (ELTs) [122]. ELTs, being non-biodegradable, pose environmental risks such as landfill overflow, fire hazards, and pest breeding [123,124]. Proper recycling addresses these issues and transforms ELTs into valuable materials [125–128], primarily rubber, which has extensive industrial uses [129,130]. However, untreated recycled rubber often has dramatically inferior properties compared to virgin rubber. Vulcanization, which enhances tire properties by creating cross-links in rubber, complicates recycling as it makes reprocessing difficult [131]. To address this, devulcanization methods are used to restore the rubber’s original form, enabling its reuse in new compounds [132–134]. Mix-

ing devulcanized and virgin rubber offers a cost-effective solution, but the property differences limit its use in high-volume, demanding applications. To meet required standards, additional processes, such as the incorporation of reinforcing additives, are necessary. This has led to the development of rubber-based composites, where (nano) particles enhance properties of recycled rubber from ELTs to approach the performance of virgin materials [135–143].

We propose a novel approach for optimal recovery of the recycled resources (here rubber from ELTs) by strategically combining additives. The study unfolds in four phases: (i) developing a semi-empirical model for property recovery compatible with physics-based machine learning, (ii) introducing a multi-objective optimization algorithm, (iii) calibrating the model with experimental data from an extensive set of experiments on filled devulcanized recycled rubber, and (iv) applying the methodology to automotive applications. This research presents a generalizable approach to recycling optimization, with the automotive case study as a benchmark, while the model is adaptable to various recycling challenges across industries.

4.2 Methods

4.2.1 Mathematical model for recovery of recycled materials

Here we formulate the recovery process for recycled materials by incorporating additives. Consider a virgin material (VM) whose number of properties of interest is N_p . Recycling this virgin material degrades its properties as:

$$P'_i = \lambda_i P_i^{(0)}, \quad i = 1, \dots, N_p \quad (4.1)$$

where $P_i^{(0)}$ and P'_i are the i -th properties of the virgin and the recycled material (RM), respectively, and λ_i is the recycling efficiency which reflects the effect of recycling on i -th properties. $\lambda_i = 1$ corresponds to the ideal case of no decrease in the properties. Here, the concept of *recovery* of an RM property is assumed as any post-treatment on the RM to decrease its deviation compared to the VM. As a solution, Additives (ADs) can be introduced in order to recover the lost portion of properties due to recycling to make a recovered recycled material, $\overline{\text{RM}}$. Considering a total number of N_a additives, the relative property of the j -th AD with respect to the RM is defined as:

$$r_{ij} = \frac{P_{ij}}{P'_i}, \quad j = 1, \dots, N_a \quad (4.2)$$

where r_{ij} is the ratio of the i -th property of j -th AD, P_{ij} , to the i -th property of the recycled material, P'_i . Note that P_{ij} is the effective property of ADs inside the RM and represents all its effects such as introducing defects and interfaces. The ratio of i -th property of $\overline{\text{RM}}$, denoted by $\bar{P}_i$, to the corresponding i -th property of VM is

defined as recovery factor,

$$\bar{R}_i = \frac{\bar{P}_i}{P_i^{(0)}}, \quad i = 1, \dots, N_p \quad (4.3)$$

The i -th recovery factor, $\bar{R}_i$, is a function, F_i , of the recycling efficiency, λ_i , the vector of the volume fractions of ADs, $\{v\}_{N_a \times 1}$, the packing configuration vector, $\{\xi_{ij}\}_{N_a \times 1}$, and the vector of ADs' property ratios for i -th property, $\{r_{ij}\}_{N_a \times 1}$, as:

$$\bar{R}_i = F_i(\lambda_i, \{v\}, \{\xi_{ij}\}, \{r_{ij}\}) \quad (4.4)$$

The deviation in the recovery of the i -th property from its virgin state, δ_i , is defined as,

$$\delta_i = |1 - \bar{R}_i|. \quad (4.5)$$

Accordingly, the overall deviation, $\bar{\delta}$, is defined as the weighted summation of the individual deviations:

$$\bar{\delta} = \sum_{i=1}^{N_p} w_i \delta_i. \quad (4.6)$$

The weights, $\sum w_i = 1$, are determined based on the importance of the corresponding deviation. By setting the weights of certain deviations to zero, it is possible to exclude them from $\bar{\delta}$. Besides, where all the deviations are of the same priority, the weights are all equal to $1/N_p$. In case all the recovery factors are equal to one, full recovery happens and the $\bar{RM}$ coincides with the VR, corresponding to no individual and thus overall deviations, $\bar{\delta} = 0$.

To represent the relative status of RM and $\bar{RM}$ compared to the VM, an N_p -dimensional Ashby plot can be employed, where each axis reflects the relative status of each property in terms of the recovery factor, $\bar{R}_i$. For the VM, all recovery factors are equal to one, while the coordinates of the RM in such an Ashby plot are determined by its given recycling efficiencies, $(\lambda_1, \dots, \lambda_{N_p})$. The more efficient the recycling process, the smaller the disparity between the VM and the RM. Figure 4.1(a) visualizes the schematic of the proposed Ashby plot in a three-dimensional Cartesian space, where the number of properties is limited to three, without sacrificing generality. As observed, incorporating ADs modifies the recovery factors through Equation (4.4). Consequently, by adjusting the volumetric fraction, packing, and the relative properties of ADs as inputs to the recovery functions, RM can enhance its recovery by minimizing deviations along a recovery path approaching VM.

Generally, the comparative space of properties in the proposed Ashby plot can be divided into 2^{N_p} sub-spaces, considering that each recovery factor can be either smaller or larger than unity and there is only one sub-space where all recovery factors, $\bar{R}_i$, are less than unity. To increase transparency, Figure 4.1(b) depicts how the division of space into these sub-spaces is accomplished in a two-dimensional Ashby plot. Besides, three schematic recovery paths are compared. In path A, the inputs

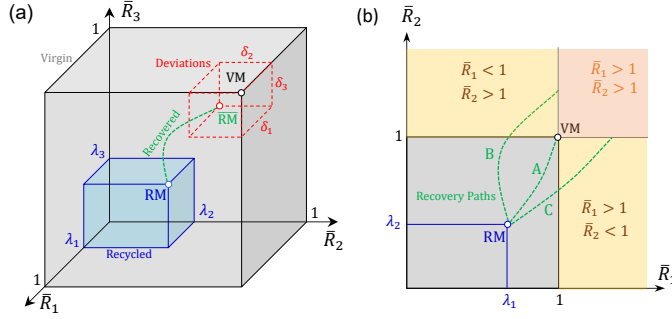


Figure 4.1. Ashby plots of the recovery process. (a) The schematic representation of the virgin material (VM), the recycled material (RM), the recovered recycled material $\overline{\text{RM}}$, and the recovery paths in a 3D Ashby plot when $N_p = 3$. (b) The schematic representation of comparative sub-spaces and different recovery paths in a 2D Ashby plot when $N_p = 2$.

of recovery functions are adjusted in a way that all properties simultaneously reach their virgin values, where the $\overline{\text{RM}}$ coincides with the VM. However, in paths B and C, the properties are fully recovered one after another. This implies that achieving complete recovery of all properties requires certain properties to surpass even those of the VM, recovery factors greater than one. The difference between *reinforcement*, i.e., $\bar{R}_i > 1$, and *recovery*, characterized by $\bar{R}_i \leq 1$, must be acknowledged. It is crucial to highlight that reinforcement may not necessarily be beneficial and it may even be deemed undesirable in certain scenarios.

The key to predicting the effect of ADs on RM, and subsequently achieving optimized recovery, lies in defining appropriate recovery functions, as introduced in Equation (4.4). In the context of heterogeneous materials, micromechanical models provide reasonable estimations for the properties of material mixtures through closed-form formulations. Among these models, the semi-empirical Halpin-Tsai (H-T) equation [144] stands out due to its successful application in predicting a wide range of properties, such as Young's modulus, Poisson's ratio, shear modulus [145], hardness [146], thermal and electrical conductivity [147], and friction coefficients [148] of mixtures. This success is attributed to its inherent fitting parameter, ξ [149]. Here, the $(N_a + 1)$ -phase version of the H-T model is customized to be used as recovery functions for N_a additives within the RM as a matrix:

$$F_i = \lambda_i \frac{1 + \sum_{j=1}^{N_a} v_j \eta_{ij} \xi_{ij}}{1 - \sum_{j=1}^{N_a} v_j \eta_{ij}}, \quad (4.7a)$$

$$\eta_{ij} = \frac{r_{ij} - 1}{r_{ij} + \xi_{ij}}, \quad (4.7b)$$

where ξ_{ij} is the fitting parameter representing the effect of the j -th AD on the i -th property. In the most general case, there are $N_a \times N_p$ independent fitting param-

eters, which may require extensive experimental and/or simulation studies to be determined. By utilizing the relationship defined in Equation (4.7), we propose a physically-informed machine learning calibration approach [150–152] to reduce the effort needed to determine the appropriate ξ_{ij} values, particularly when multiple ADs interactively contribute to the recovery function, as illustrated schematically in Figure 4.2.

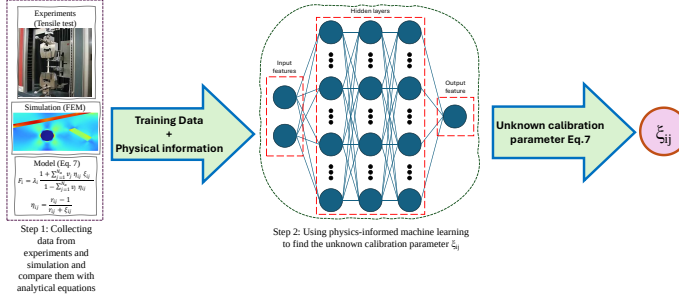


Figure 4.2. The schematic of proposed physically-informed machine learning approach. It takes the inputs from experiments/simulations and provides the calibrated fitting parameters, $[\xi]_{N_p \times N_a}$, while physically informed by the recovery model offered in Equation (4.7).

The H-T version of the recovery functions can be converted to either the direct rule of mixtures (ROM) or the inverse rule of mixtures (IROM) by setting the fitting parameter in Equation (4.7) to infinity or zero, respectively [144]. The ROM version, which is a linear weighted summation, provides an upper bound for the effect of ADs on properties, as follows:

$$F_i = \lambda_i \left(1 + \sum_{j=1}^{N_a} (r_{ij} - 1) v_j \right) \quad (4.8)$$

Despite its simplicity, the ROM provides accurate predictions in certain cases, such as Young’s modulus when the ADs are in the form of long fibers aligned in the direction of the applied load [153]. Additionally, Equation (4.8) can be utilized to calculate the relative cost of the mixture compared to the matrix, where the total price is simply a linear weighted summation of the prices of the components. Thus, one can deduce from Equation (4.8) that,

$$F_{\S} = \lambda_{\S} \left(1 + \sum_{j=1}^{N_a} (r_{\S j} - 1) v_j \right) \quad (4.9)$$

where $F_{\S}$ is the cost ratio of $\overline{\text{RM}}$ to VM (recovered to virgin), $\lambda_{\S}$ is the cost ratio of RM to VM (recycled to virgin), and $r_{\S j}$ is the cost ratio of the j -th AD to RM (additive to recycled).

In contrast to ROM, the IROM version of the recovery function provides the lower bound for the effect of ADs on the property of the matrix. It is reported that this simple micromechanics formulation provides an acceptable estimation for some properties of mixtures of materials such as transverse Young's modulus of aligned ADs perpendicular to the load direction [153], or friction coefficients of mixtures [154]. The recovery function based on the IROM model is obtained by setting $\xi_{ij}=0$ in Equation (4.7) as,

$$F_i = \frac{\lambda_i}{\left(1 + \sum_{j=1}^{N_a} \left(\frac{1}{r_{ij}} - 1\right)v_j\right)}, \quad (4.10)$$

After defining the recovery problem, the next step is to solve it. This involves identifying the appropriate types of ADs and determining their corresponding volume fractions to achieve the target property deviations. To establish a foundational understanding, consider the simplest case where there is only one AD to recover one property of interest, i.e., $N_a = N_p = 1$. By substituting the recovery function from Equation (4.7) into the deviation function, Equation (4.5), the volume fraction can be obtained as a function of the deviation, $\bar{v}$, as,

$$\bar{v}(\delta_1) = \frac{\frac{1-\delta_1}{\lambda_1} - 1}{\eta_{11} \left(\xi_{11} + \frac{1-\delta_1}{\lambda_1}\right)}, \quad (4.11)$$

where $\eta_{11} = (r_{11} - 1)/(r_{11} + \xi_{11})$. The critical volume fraction of AD, $\bar{v}_{cri}$, which causes full recovery, can then be determined by setting the deviation to zero in Equation (4.11),

$$\bar{v}_{cri} = \frac{\frac{1}{\lambda_1} - 1}{\eta_{11} \left(\xi_{11} + \frac{1}{\lambda_1}\right)}. \quad (4.12)$$

Now, let us expand this idea to the case where the number of properties and the number of ADs increases. In this case, each AD has the potential to influence all the investigated properties through the ratio vectors $\{r_{ij}\}$. Considering a deviation δ_i from the VM for each property, by inserting the N_p recovery functions from Equation (4.7) (or its simplified versions in Equation (4.8) and Equation (4.10)) into Equation (4.5), a system of algebraic equations in the following matrix expression is obtained:

$$[A]_{N_p \times N_a} \{\bar{v}\}_{N_a \times 1} = \{b\}_{N_p \times 1}. \quad (4.13)$$

The elements on the i -th row of the matrix, $[A]$, specify the efficacy of N_a ADs in the recovery of the i -th property, while the element of the vector $\{b\}$ are defined using the predefined deviation, δ_i , and the corresponding recycling efficiency, λ_i . The components A_{ij} , and b_i are presented in Table 4.1 for H-T, ROM, and IROM recovery functions. Note that when $\delta_i = (1 - \lambda_i)$, then, $b_i=0$, corresponding to no recovery (RM and $\bar{RM}$ coincide in Figure 4.1(a)). Regarding the algebraic system of equations, three distinct scenarios may arise depending on the comparison between the number of ADs, N_a , and the number of properties considered for recovery, N_p :

Table 4.1. The elements A_{ij} of the matrix $[A]$ and b_i of the vector $\{b\}$ in Equation (4.13) where $i = 1, \dots, N_G$ and $j = 1, \dots, N_a$.

	A_{ij}	b_i
H-T	$\eta_{ij} \left(\xi_{ij} + \frac{1-\delta_i}{\lambda_i} \right)$	$\frac{1-\delta_i}{\lambda_i} - 1$
ROM	$r_{ij} - 1$	$\frac{1-\delta_i}{\lambda_i} - 1$
IROM	$1 - \frac{1}{r_{ij}}$	$1 - \frac{\lambda_i}{1-\delta_i}$

Scenario one, $N_a = N_p$: There are exactly enough ADs to recover all the properties. Consequently, the matrix $[A]$ becomes a square matrix, and a unique vector for the volume fraction can be determined as a function of predefined deviations as follows:

$$\{\bar{v}\} = [A]^{-1}\{b\}. \quad (4.14)$$

Solving Equation (4.14) requires the inverse of the matrix $[A]$, which has dimensions $N_a \times N_p$. Then, one can insert $\{\bar{v}\}$ into Equation (4.9) to obtain the cost ratio of recovery, F_g , as a function of deviations, and consequently assess the cost ratio for full recovery by setting the deviations to zero. **Appendix D.1** provides the closed-form equations for determining volume fractions as a function of deviations in the simplest multi-AD recovery scenario, where the number of recovery properties equals the number of additives (both set to 2). This is complemented by **Appendix D.2**, which presents a parametric study to analyze the effects of various parameters on recovery performance.

Scenario two, $N_a > N_p$: The number of ADs exceeds the number of properties, resulting in more unknown volume fractions than available equations. In this case, incorporating extra ADs can expand recovery options and enhance decision-making. This flexibility proves particularly advantageous in actual manufacturing conditions where factors such as market availability or complexities in the mixing process impose real-world constraints. With more ADs available than properties to recover, these extra ADs, denoted as ADs⁺, introduce extra degrees of freedom in problem-solving. It is important to note that while this surplus enables more recovery options, it may also increase costs. When $N_a > N_p$, the system of equations in Equation (4.13) has more variables than equations, resulting in infinite solutions rather than a unique one. To achieve a unique solution, one approach is to designate a specific number of ADs (equal to the difference between N_a and N_p) as supplemental ADs with predefined fixed volume fractions, $\{\bar{v}\}^+$. This adjustment restores the squareness of the matrix $[A]$, enabling the use of Equation (4.14) to determine the volume fractions of the remaining ADs. **Appendix D.3** provides a case study illustrating how increasing the number of ADs can diversify choices for solving a recovery problem.

Scenario three, $N_a < N_p$: There are more properties to recover than available ADs. As a result, it may not be feasible to find a solution for Equation (4.13). The only feasible approach to finding a solution is to engineer additives such that they can simultaneously recover multiple properties to achieve their desired deviations. This consolidation results in some recovery equations in the system of algebraic equations becoming dependent and being eliminated, thereby allowing the matrix $[A]$ to become square and invertible again. Subsequently, the volume fraction vector corresponding to the desired deviations can be determined using Equation (4.14).

An extreme case of *scenario three* is to exclusively design a single AD for a specific recovery problem where adding a certain volume fraction of this AD enables the recovery of all investigated properties to reach the target deviations simultaneously. For a single AD ($N_a=1$) recovering N_p properties, the matrix form of the recovery problem in Eg. Equation (4.13) is simplified as,

$$v_1 \begin{bmatrix} A_{11} \\ \vdots \\ A_{N_p,1} \end{bmatrix} = \begin{Bmatrix} b_1 \\ \vdots \\ b_{N_p} \end{Bmatrix}. \quad (4.15)$$

Simultaneous recovery of all properties is feasible by adding the predefined chosen volume fraction, v^* , if the relationship between the elements of b_i and A_{i1} remains consistent across all properties:

$$\frac{b_i}{A_{i1}} = v^* \quad i = 1, \dots, N_p \quad (4.16)$$

From a linear algebra perspective, Equation (4.16) condenses the N_p system of equations into a single independent equation that satisfies all properties simultaneously. Indeed, Equation (4.16) imposes a restriction to all influencing parameters including ratios of the properties of AD to RM, r_{i1}^* , the recovery efficiencies of properties, λ_i , and the targeted deviations, δ_i . The exclusively designed single AD should be engineered to satisfy the relationship dictated by Equation (4.16). The critical predefined volume fraction of the engineered AD, v_{cri}^* , which ensures full recovery of all properties simultaneously, can be determined by setting all the deviations to zero while evaluating the coefficients b_i in Equation (4.16). A sample case study on designing such a single AD is presented in **Appendix D.4**.

4.2.2 Establishing the optimization framework for recovery

Here, we describe the setup of the optimization problem for recovering a recycled material using ADs. This includes defining the pre-defined input data, specifying the objective functions, and outlining any constraints that may apply.

required input information:

- The vector of recycling efficiencies of N_p properties under examination (recycled to virgin), $\{\lambda\}_{N_p \times 1}$.
- The cost ratio of RM to VM (recycled to virgin), $\lambda_{\S}$.
- The N_p vectors of the property ratio of the ADs to RM (additive to recycled), $\{r_{ij}\}_{N_a \times 1}$
- the N_p vectors of the packing fitting parameter of the ADs, $\{\xi_{ij}\}_{N_a \times 1}$
- The vector of the cost ratio of the ADs to RM (additive to recycled), $\{r_{\S j}\}_{N_a \times 1}$.

Possible objective functions to be minimized:

- The individual deviations from the VM, δ_i , as defined in Equation (4.5), ideally zero for full recovery of that property.
- The overall deviation, $\bar{\delta}$, as defined in Equation (4.6), ideally zero for full recovery of all the properties.
- The relative cost of the recovery, $F_{\S}$, as defined in Equation (4.9). the smaller the $F_{\S}$ value, the more cost-effective the recovery becomes. In the extreme case where $F_{\S}=1$, the price of $\overline{\text{RM}}$ equals that of VM, and for $F_{\S} > 1$, the economic justification for the recovery process diminishes.

Possible constraints:

- Constraints on the volume fraction vector: A Constraint can be defined on the total volume fraction of ADs, either via setting a certain total volume fraction, v_T , or setting two maximums and minimums scalars, $(v_T)_{min}$ and $(v_T)_{max}$. Note that the former applied to the total volume fraction is a linear constraint as the summation of the volume fraction of ADs, while the latter imposes nonlinear constraints in the form of inequalities. Additionally, the constraints may be applied as the pairs of maximums and minimums on every individual AD which can be presented via two constrain vectors, $\{v\}_{min}$, and $\{v\}_{max}$ of size $N_a \times 1$.
- Constraints on recovery deviations: It can be applied either as a vector of maximum allowable deviations, $\{\delta\}_{max}$ of size $N_p \times 1$, or as a maximum overall allowable deviation, $(\bar{\delta})_{max}$.

The output of the optimization algorithm is the tuned vector of volume fraction of ADs, $\{v\}_{opt}$, and the corresponding values of the objective functions while satisfying predefined constraints.

From a multi-objective (MO) optimization perspective, a set of N_g objective functions can be defined, with the corresponding Pareto fronts determining the optimal solution space. Figure 4.3 presents the schematic of the optimization algorithm for optimal recovery.

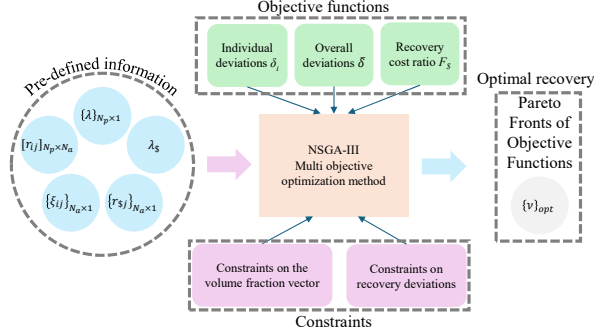


Figure 4.3. The schematic of multi-objective optimization algorithm for optimal recovery of RM. The pre-defined information is required as the input. The output is the Pareto Fronts of objectives and the corresponding volume fraction of ADs, while satisfying the imposed constraints on the volume fractions and deviations.

4.2.3 The numerical implementation of the MO optimization algorithm

NSGA-III (Non-dominated Sorting Genetic Algorithm III) is a high-dimensional multi-objective optimization algorithm that uses reference points to maintain diverse solutions along the Pareto front [155, 156]. Implemented in Julia through the Metaheuristics package, it capitalizes on Julia's speed and efficiency for complex optimization tasks [157]. In our study, a population of 2000 was used, and the algorithm ran for 1000 iterations to ensure a well-distributed Pareto front, addressing trade-offs between multiple objectives effectively. The validation study for the optimization algorithm is presented in **Appendix D.5**.

4.2.4 Experimental measurements of the properties of the virgin rubbers VM1 and VM2 and their blends with recycled rubbers SRC0 to SRC9

To determine the optimal replacement of VMs with SRCs, it is crucial to understand how this substitution affects the material properties. For VM1, the focus is on six properties: hardness, tensile strength, elongation at break, modulus of elasticity (at strain 100%), tear strength, and compression set. In contrast, for VM2, the evaluation includes four properties: tensile strength, elongation at break, modulus of elasticity at strain 100%, and toughness (the area under the stress-strain curve). In [158], we proposed a detailed micromechanical model for evaluating the impact of nano-filled SRCs on a VM. However, in this study, we adopt a direct experimental measurement approach. This methodology is chosen to bypass the uncertainties associated with interphase properties and other unknown variables inherent in micromechanical

modeling. By relying on empirical data, we aim to provide an accurate and realistic assessment of the effective modification in the properties of the VMs with SRC additions, thereby inherently integrating all relevant factors such as interphases and defects introduced during the blending. To evaluate the impact of incorporating SRCs on the specified properties of interest, we first measure these properties for two VMs without any SRC addition. Subsequently, we introduce a specific volume fraction of each SRC into the virgin materials—20% for VM1 and 10% for VM2—and measure the properties again. We then compute the ratio F_i of the properties of the mixture (VMs plus SRCs) to the corresponding properties of the VM by dividing the measured values. **Figure D.5** (a) and (b) illustrate the F_i ratios for the properties of VM1 and VM2, respectively. These experimental measurements reveal that the incorporation of SRCs into VMs leads to a diverse spectrum of property modifications. These changes include both enhancements and degradations, depending on the specific SRC and property in question. Nonetheless, due to the intrinsic nature of recycled materials, the addition of SRCs generally results in a degradation of material properties.

For each SRC added to the VM, we insert the measured F_i values and the corresponding volume fraction (0.2 for VM1 and 0.1 for VM2) into Equation (4.7). Since there is only one added SRC per mixture, $N_p = 1$. Additionally, given that the matrix is composed of VM, the recycling efficiency is 100%, i.e., $\lambda_i = 1$. The remaining two values in the recovery function, Equation (4.7), are the property ratio r_{ij} and the fitting parameter ξ_{ij} . Ideally, the properties of the individual SRCs should also be measured separately, allowing for the calculation of r_{ij} ratios. By inserting r_{ij} , the recovery equations for each property and each blend can be fit to the experimental data to determine the values of the fitting parameters ξ_{ij} . This fitting process can be conducted using a physically-informed machine-learning approach similar to that depicted in Figure 4.2. However, the process faces the challenge of a large number of blends and properties to be evaluated. Specifically, here we have a total of 20 blends (combinations of ten SRCs with the two VMs), and six and four properties are of interest, respectively for VM1 and VM2. This results in a total of 100 different recovery functions, necessitating the fitting process to determine 100 fitting coefficients ξ_{ij} , making the fitting process practically infeasible. To overcome, here we make a reasonable assumption for fitting parameter: it is assumed that the SRCs are distributed homogeneously and randomly within the VM as semi-spherical particles by setting the H-T fitting parameter for all blends and all properties equal to $\xi_{ij} = 2$ [158]. Then, we solve Equation (4.7) for r_{ij} to back-calculate the ratio of the properties of the j -th SRC to the i -th properties of VMs. In this way, we derive the ratio of the *effective* properties of each SRC when blended with the VMs, considering all effects such as interface formation or potential defects. Consequently, these r_{ij} values are more practical compared to directly measuring the properties of SRCs and dividing them by the properties of VM since it accounts for possible inaccuracies associated with assuming $\xi_{ij} = 2$ for all properties, providing a more accurate representation of the SRC's impact on the VM. The total 100 calculated r_{ij} values for the two virgin materials, VM1 and VM2, are presented in **Table D.3** and **Table D.4**, respectively.

When $r_{ij} = 1$, the property of the SRC is equivalent to that of the VM. Conversely, $r_{ij} > 1$ and $r_{ij} < 1$ signify that the SRC has superior and inferior properties compared to the VM, respectively.

It should be noted that although the same SRCs have been added to both VM1 and VM2, their effects on the same property can differ significantly. A primary reason for this is the intrinsic differences in the compositions of the two virgin materials. VM2, which is utilized in tire production, has a markedly different composition compared to VM1, which is used in the manufacture of spring pads in automotive suspension systems. VM2 inherently contains a substantial proportion of various additives, including carbon black and sulfur, which can significantly influence the efficacy of the SRCs. These additives are designed to enhance specific properties required for tire performance but may interact differently with the SRCs compared to the relatively simpler composition of VM1. Additionally, the process parameters involved in blending SRCs with VMs vary and can affect the final impact of SRCs on the material properties. For instance, when comparing column $i = 2$ in **Table D.3** with column $i = 1$ in **Table D.4**, it becomes evident that the addition of SRCs impacts the tensile strength of VM1 and VM2 differently, resulting in distinct r_{ij} ratios.

During the back-calculation, negative values for r_{ij} may be encountered, as seen in **Table D.3** and **Table D.4**. To interpret these values, it is essential to understand that for a void introduced to the VM, $r_{ij} = 0$. Hence, a negative r_{ij} suggests that the addition of the SRC has a more degradation effect on the properties of the VM than if an equivalent volume fraction of voids were introduced into the VM. Lastly, it is noted that the r_{ij} ratios are calibrated based on experimental test results involving the combination of a single SRC with the VMs. Consequently, applying these ratios to blends containing multiple SRCs does not account for potential interactions among the SRCs.

4.3 Results

4.3.1 The targeted virgin and recycled resources

Since the automotive industry is under increasing pressure to adopt more sustainable practices [159], here we explore the feasibility of partially replacing virgin rubbers in two key sectors [160]: the production of spring pads in suspension systems, and passenger car tires, referred to as VM1 and VM2, respectively provided by Stellan-tis [161] and Bridgestone [162]. These components are not only mass-produced but also represent a substantial share of global raw rubber consumption. We utilize a devulcanized recycled rubber from ELTs, referred to as SRC0, provided by Rubber Conversion srl, Italy [163]. SRC0 is then combined with nine different nanofillers, resulting in nine new nano-filled RM, labeled SRC1 through SRC9. The incorporation of nanofillers significantly modifies the properties of SRC0, thus creating a diverse set of ten choices of replacement with distinct characteristics. The primary objective is

to ensure that the final properties of this rubber blend (partial replacement of VM1 or VM2 with SRCs) meet the required technical standards. Such an initiative not only promotes sustainable material usage but also reduces the dependency on natural and synthetic rubber. This strategy can lead to significant environmental and economic benefits by lowering raw material consumption and minimizing waste. The current scenario of *replacement* of SRCs within the VMs involves a matrix composed of a VM, whose properties are inherently optimal and do not require recovery. The objective, driven by economic and environmental considerations, is to replace a targeted fraction of the VM, v_T , with SRCs. Here, SRCs act as additives (ADs) not as reinforcements, since they are (nano-filled) recycled ELTs. As a consequence, the replacement of VMs with SRCs potentially causes deviations from the properties of the VMs. In this context, the proposed model and the associated optimization algorithm are employed to determine the optimal replacement strategy that minimizes costs while effectively minimizing and controlling deviations in properties. This approach ensures that the final rubber blend retains desirable characteristics, promoting the sustainable use of ELTs without compromising performance. Note that it is different from the case studies presented in the **Appendix D.2 and Appendix D.5**, where the base material (matrix) was an RM with efficiency lower than VM, and ADs were used as reinforcements to *recover* the properties of RM, reducing its deviation from VM.

For the cost-benefit analysis, it is essential to establish the relative pricing of these SRCs in comparison to VMs. It is assumed that the neat devulcanized recycled rubber, SRC0, which does not contain any nanofillers, is priced at 50% of the cost of either VM1 or VM2, whereas SRC1 to SRC9, which include various nanofillers, are priced equivalently to VM1 and VM2. This reflects the fact that the additional expense incurred from the nanofillers offsets the lower cost of the base SRC0 material. From a cost perspective, substituting VM1 or VM2 with any of the SRC1 to SRC9 does not offer cost savings and SRC0 remains the only cost-effective option for achieving cost reduction while utilizing recycled materials. It is emphasized that cost reduction is not the primary goal of substituting VMs with SRCs. Even if the substitution does not lead to a considerable decrease in the final cost of the product, the incorporation of SRCs into the production cycle represents a significant achievement supporting resource conservation and the sustainable use of recycled materials.

4.3.2 Case Study: Optimal replacement of recycled ELTs within the virgin rubbers

Here, we examine the replacement of 20% of the virgin rubbers VM1 and VM2 with SRCs. To ensure that this replacement objective is consistently met, we impose a fixed constraint on the volume fraction of SRCs across all results, $v_T = 0.2$. We explore two optimization approaches to determine the optimal recovery strategy: the first involves a three-objective optimization without constraints on property deviations,

while the second involves a two-objective optimization with constraints applied to property deviations.

In the three-objective optimization, the objective functions are defined as follows: The first objective function is the ratio of the blend price to the price of the virgin rubber, $F_{\S}$. Among the SRCs, only SRC0, can reduce the blend price relative to VMs. Since it is assumed to cost half as much as both VMs, $F_{\S}$ ranges between 0.9 and 1, where 0.9 represents the minimum price, when SRC0 fills the entire 20% of replacement, and 1 represents the maximum price, when no SRC0 is used, see Equation (4.9) in the Section 4.2. The second objective function is the overall deviation, $\bar{\delta}$ defined in Equation (4.6) in the Section 4.2, which reflects the average performance of the blend compared to VMs. A deviation of zero indicates that the blend's properties match those of VMs exactly. To evaluate the overall deviation, the properties are assigned equal weights, with VM1 properties receiving a weight of $\frac{1}{6}$ and VM2 properties $\frac{1}{4}$, corresponding to the six and four properties of interest for VM1 and VM2, respectively. The third objective function focuses on the deviation of every individual property, δ_i , see Equation (4.5) in the Section 4.2. This allows the optimization process to not only minimize the cost and overall performance deviation compared to VMs but also to target and reduce deviations in a specific property. Thus, the optimization approach aims to balance cost reduction with overall performance improvement and specific property enhancements.

This choice of objective functions leads to six independent optimizations for VM1 and four for VM2. For each optimization study, the Pareto front of the three objective functions is illustrated as a three-dimensional plot in the Cartesian coordinate system $(F_{\S}, \bar{\delta}, \delta_i)$. This plot represents a range of optimal solutions, capturing the trade-offs among these three objectives. Additionally, for each displayed Pareto front, the volume fractions of the corresponding SRCs at the boundaries (edges of the 3D surface) are provided. This information helps determine which SRCs should replace 20% of the VMs for each optimal point on the Pareto front.

Figure 4.4(a)-(f) shows the Pareto fronts and the corresponding volume fractions of SRCs for optimal replacement with VM1 for six properties of interest. In all scenarios, point A, corresponds to the lowest price, $F_{\S}=0.9$. At this point, as expected, the optimization algorithm has replaced the entire 20% with SRC0. However, the exclusive use of SRC0 does not necessarily result in the lowest overall deviation, nor does it lead to the lowest deviation for the specific property being investigated. Therefore, to optimize these deviations, other SRCs must be utilized, which increases the cost. This is evident from the gradual decrease in the volume fraction of SRC0 (blue areas in the volume fraction diagrams) as the solution moves away from point A. Since SRC0 is not the best option for reducing the deviation for any of the properties, at the points where deviations reach their absolute minimum values, for example, the BC edge in Figure 4.4(a), SRC0 may not be included in the replacement. Consequently, the price of the blend could reach the price of VM1, i.e., $F_{\S}=1$.

In general, it can be observed that in all six optimal replacements, SRC3 frequently emerges as a significant alternative for reducing deviations since it exhibits acceptable performance across all six properties on average. Therefore, the optimiza-

tion algorithm is more likely to select it to minimize the overall deviation $\bar{\delta}$. However, when the focus shifts towards achieving the absolute minimum for any specific δ_i deviation, the optimization algorithm tends to allocate a larger share to the SRC that most closely matches the performance of VM1 in that particular property. For instance, for minimizing deviations in hardness, tensile strength, and tear strength, the algorithm assigns higher volume fractions to SRC9, SRC1, and SRC8, respectively, as approved by r_{ij} values in the **Table D.3**.

Regarding the elastic modulus in Figure 4.4(d), although SRC5 exhibits a slightly higher elastic modulus compared to SRC1, both SRCs serve as the suitable choice in bringing the blend elastic modulus closer to VM1. However, their effects on other properties are markedly different and sometimes even opposite. For instance, SRC1 shows the weakest performance in tear strength, whereas SRC5 underperforms in hardness and elongation. In such scenarios, the optimization algorithm smartly employs a combination of SRC1 and SRC5 in specific proportions to enhance the elastic modulus while simultaneously minimizing the overall deviation. This balanced approach ensures that the blend maintains desirable properties across multiple attributes, optimizing the overall performance. A similar interpretation applies to the combination of SRC0, SRC1, and SRC7 in minimizing the deviation in elongation. While both SRC1 and SRC7 exhibit acceptable performance in elongation, comparable to VM1, they both perform poorly in terms of elastic modulus. To address this, the optimization algorithm incorporates SRC2 into the mixture to compensate for the deficiencies in modulus, thereby achieving a balanced improvement across multiple properties.

Lastly, it is noticeable that although SRC1 and SRC9 have compression sets closest to VM1, the optimization algorithm unexpectedly selects a combination of SRC4 with SRC3 and SRC0 to minimize the deviation. This decision arises because SRC0 and SRC3, which are optimal for minimizing cost and overall deviation, respectively, both exhibit higher compression set values than VM1 (91% and 15%, respectively). Therefore, the algorithm opts to retain SRC0 and SRC3 while incorporating SRC4, which has a compression set of 61% of that of VM1, into the blend to effectively minimize the deviation δ_6 .

Figure 4.5(a)-(d) presents the results of four three-objective optimizations for combining SRCs with VM2, depicted as four Pareto fronts along with the corresponding volume fractions of SRCs at the boundaries of these surfaces. In these optimizations, the algorithm predominantly utilizes SRC0 and SRC2 to minimize F_s and $\bar{\delta}$, respectively. For the properties of elongation and toughness, SRC6 is added as a third contributor. For tensile strength, again SRC6 is included as the third SRC, however, a low percentage of SRC1, the highest tensile strength among the SRCs, is added. Regarding the elastic modulus, since SRC0, as the most cost-effective choice, also provides the highest modulus, the algorithm prefers to easily combine it with SRC2 to minimize overall deviation. Interestingly, in some cases, a small amount of SRC7 is present in the optimal combination despite its overall weak properties. This occurs because the optimization algorithm aims to minimize both positive and negative deviations. Given that the elastic modulus of SRC0 is much higher than that of VM2,

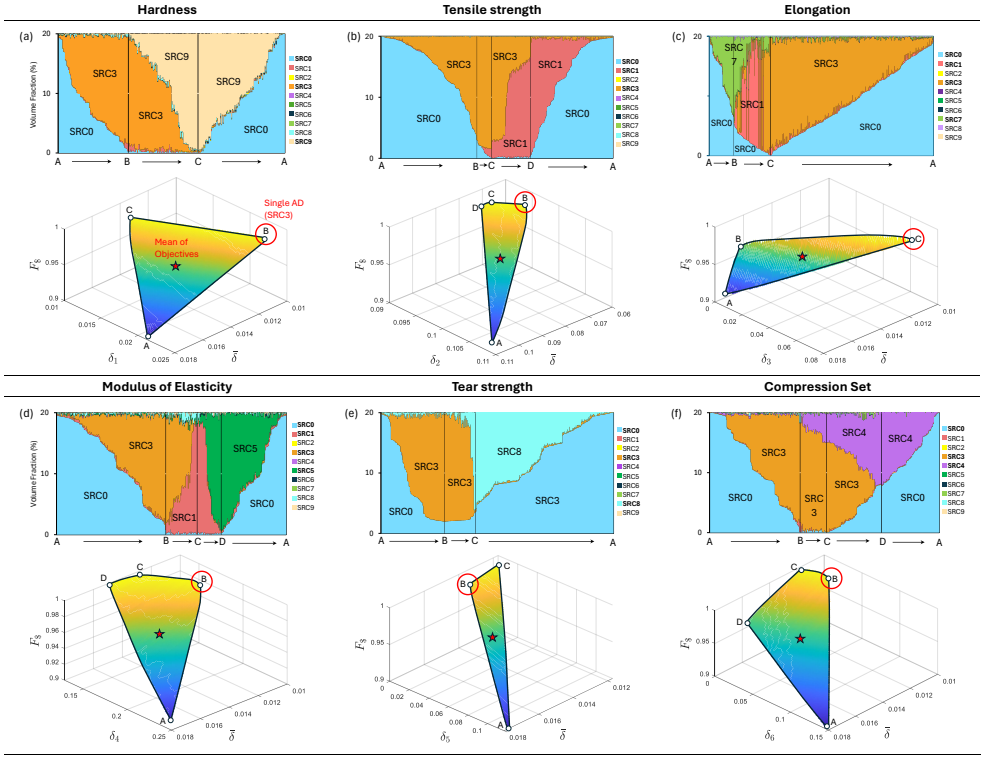


Figure 4.4. The three-objective optimization of the replacement of 20% of VM1 with SRCs for the six properties of interest focusing on every individual property. The objective functions are the cost ratio of blend compared to the VM1, $0.9 < F_s < 1$, the overall deviation of the six properties calculated from Equation (4.6) (in the Section 4.2) with the same weight of $w_i = \frac{1}{6}$, and the deviation of the individual under focuses property. The 3D surface representations of the Pareto fronts of objective functions are presented for every optimization study. Besides, the corresponding volume fractions of the contributing SRCs are presented on the boundary of Pareto fronts.

achieving minimum deviation requires adding a fractional amount of SRC7 to better match the stiffness of VM2. The algorithm also intelligently excludes SRC3, SRC4, SRC5, SRC8, and SRC9 from the optimal replacement combinations, as at least one of the r_{ij} values for these SRCs is too low, indicating suboptimal performance in the desired properties.

After presenting the three-objective optimizations, a set of two-objective optimizations is introduced where the cost ratio, F_s , and overall deviation, δ , are chosen as the objective functions. To focus on the deviation of specific properties, a constraint is defined as $\delta_i < \delta_{i,\max}$. Unlike the three-objective studies, which aim to minimize the δ_i deviation, the goal here is not necessarily to minimize δ_i but to find the optimal

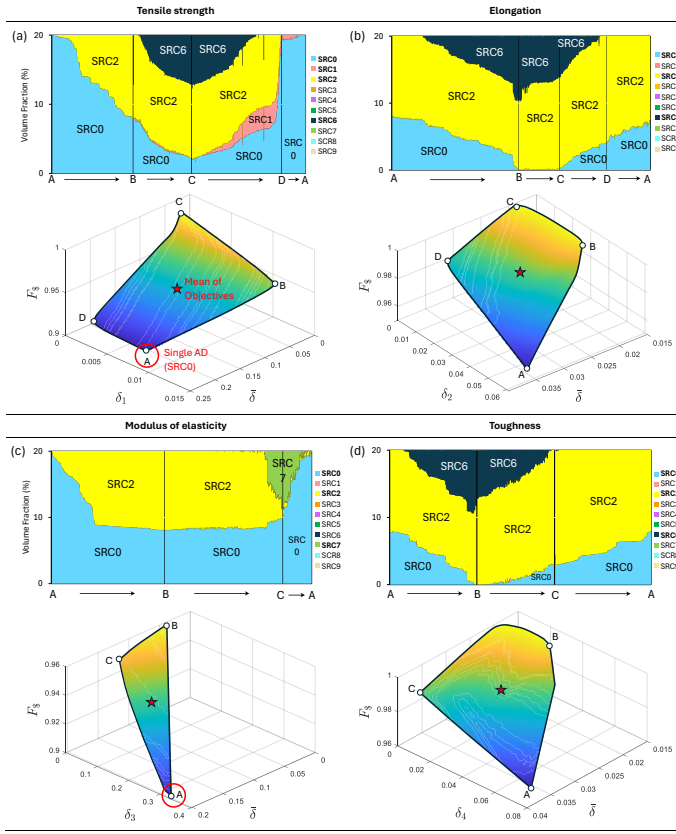


Figure 4.5. The three-objective optimization of the replacement of 20% of VM2 with SRCs for the four properties of interest focusing on every individual property. The objective functions are the cost ratio of blend compared to the VM2, $0.9 < F_s < 1$, the overall deviation of the four properties calculated from Equation (4.6) (in the Section 4.2) with the same weight of $w_i = \frac{1}{4}$, and the deviation of the individual under focuses property. The 3D surface representations of the Pareto fronts of objective functions are presented for every optimization study. Besides, the corresponding volume fractions of the contributing SRCs are presented on the boundary of Pareto fronts.

solutions for F_s and $\bar{\delta}$ that satisfy the δ_i constraint. The value of the constraint $\delta_{i,\max}$ represents the maximum acceptable deviation for the i -th property. This value is typically defined by design standards and operational considerations. The stricter the constraint (i.e., $\delta_{i,\max}$ closer to zero), the more challenging it becomes to find optimal solutions, and the more limited the Pareto front is. If, under stringent conditions, all SRCs for a property are weaker than the VMs (all r_{ij} are less than one), tightening the constraint further may result in no feasible solutions. To systematically explore this, we apply constraints on each investigated property for VM1 and VM2 one at

a time, gradually tightening the constraint towards zero until the algorithm fails to find a feasible Pareto front. This process helps identify the SRCs that play the most crucial role in meeting the constraint within the blend.

Constrained two-dimensional optimizations for a 20% replacement of SRCs within VM1 are illustrated through the volume fractions of SRCs used (Figure 4.6(a)-(g)), and the corresponding 2D Pareto fronts (Figure 4.6(h)). Initially, in Figure 4.6(a), no constraint is applied to any of the six properties where the optimization algorithm selects SRC0 and SRC3 to minimize F_s and $\bar{\delta}$, respectively. As observed in the corresponding Pareto front, moving from point A to point B, the share of SRC0 increases, and the overall deviation $\bar{\delta}$ gradually increases while F_s approaches its minimum at 0.9.

For hardness with the condition $\delta_1 < 0.015$, the algorithm selects SRC1 to satisfy this constraint. However, in the corresponding three-objective optimization where hardness was the third objective function (see Figure 4.4(a)), SRC9 was chosen to minimize δ_1 . This illustrates the difference between applying even a strict constraint on a property and aiming to minimize that property. When the algorithm seeks to achieve the absolute minimum deviation in a property (the state closest to the VMs), it tends to select the SRC with the highest performance in that property (the highest r_{ij}), as seen in the case of SRC9 for hardness. Conversely, when a constraint is applied to the deviation of a property, the algorithm prefers the SRC that, while satisfying the constraint, maximizes the overall effectiveness in minimizing both the overall deviation and cost. For tensile strength, elastic modulus, and tear strength, when constraints $\delta_2 < 0.095$, $\delta_4 < 0.14$, and $\delta_5 < 0.001$ are applied, SRC1, and SRC8, which exhibit the best performance in these properties, emerge in the optimal combination. These selections align with the results from the three-objective optimization. The similarity in the choices can be attributed to SRC1 and SRC8, which, despite not having the maximum r_{ij} in other properties, still offer acceptable performance overall. Regarding the elongation at break, since the most cost-effective choice, SRC0, has a very close performance to VM1, the algorithm consistently allocates a major part of the optimal combination to it. To adjust the overall deviation and satisfy the constraint $\delta_3 < 0.01$, a combination of SRC3 and SRC7, similar to the strategy observed in the corresponding three-objective optimization, is used. Applying the constraint $\delta_6 < 0.005$ on the compression set results in the addition of SRC4 to the optimal replacement combination, exactly as seen in the three-objective optimization in Figure 4.4(f). As mentioned, SRC4, with a compression set equal to 61% of VM1, is added to moderate the high values of this property for SRC0 and SRC3, thereby bringing it closer to VM1. Among all constraints, the least stringent one is applied to the elastic modulus, $\delta_4 < 0.14$, resulting in the greatest deviation from VM1. This observation is supported by the data in the **Table D.3**. While for other properties there are SRCs with performance that closely approximate VM1 (indicated by r_{ij} values near one), the best-performing SRC for the elastic modulus, SRC1, remains substantially distant from VM1.

Similarly, Figure 4.7 illustrates the optimal combinations and the corresponding Pareto fronts for the constrained two-objective optimization involving a 20% replace-

ment of SRCs in VM2. In the unconstrained scenario, the optimal combination consists of SRC0, SRC2, and SRC6, which effectively minimize both the cost ratio, F_s , and the overall deviation, $\bar{\delta}$. When constraints are applied to elongation, elastic modulus, and toughness with $\delta_2 < 0.002$, $\delta_3 < 0.01$, and $\delta_4 < 0.001$, the algorithm selects the same three SRCs, although in different proportions compared to the unconstrained case, resulting in a higher price but achieving the desired performance. For tensile strength, the algorithm also includes SRC4 in the optimal combination.

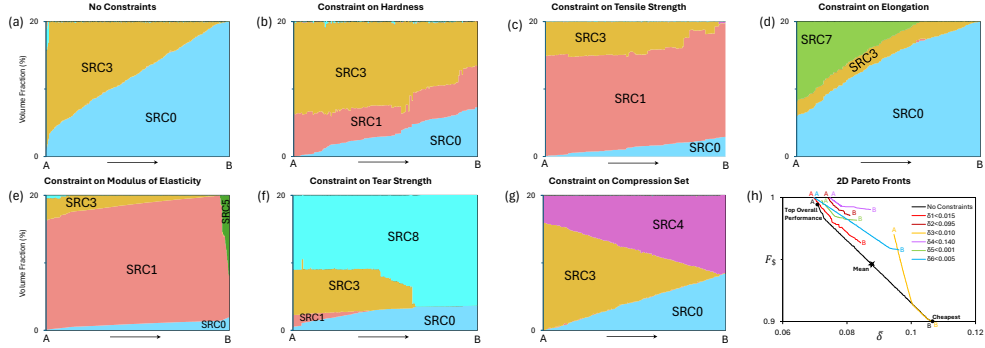


Figure 4.6. The two-objective optimization of the replacement of 20% of VM1 with SRCs imposing constraints on the six properties of interest. The two objective functions are the cost ratio of blend compared to the VM1, $0.9 < F_s < 1$, and the overall deviation of the six properties calculated from Equation (4.6) (in the Section 4.2) with the same weight of $w_i = \frac{1}{6}$. The 2D Pareto fronts and the corresponding volume fraction of the SRCs for an optimized replacement are presented.

In both Figure 4.6 and Figure 4.7, a comparison of the constrained and unconstrained Pareto fronts reveals that the constrained solutions are unable to achieve the minimum cost and overall deviation. This limitation arises because the constraints necessitate the inclusion of alternative SRCs, which prevents reaching the optimal cost associated with SRC0. Consequently, the constrained Pareto fronts are shorter compared to their unconstrained counterparts. However, as the constraints on δ_i are progressively relaxed, the constrained Pareto fronts gradually converge toward the unconstrained ones. This shift occurs because allowing individual properties to deviate more from the VMs. Therefore, the volume fractions of SRCs in optimal combinations approach the unconstrained solutions in Figure 4.6(a) and Figure 4.7(a) for VM1 and VM2.

4.4 Discussion

After a detailed discussion on the outputs and the capabilities of the proposed optimization algorithm in the **Section 4.3**, we outline the material selection process followed during the project [160] for integrating SRCs into VM1 and VM2 virgin rub-

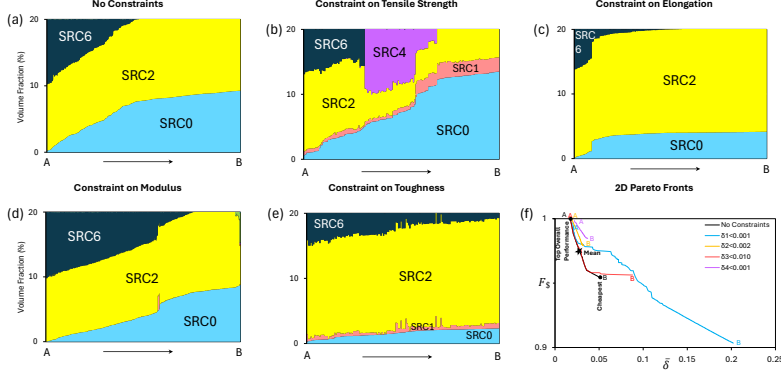


Figure 4.7. The two-objective optimization of the replacement of 20% of VM2 with SRCs imposing constraints on the four properties of interest. The two objective functions are the cost ratio of blend compared to the VM1, $0.9 < F_s < 1$, and the overall deviation of the four properties calculated from Equation (4.6) (in the Section 4.2) with the same weight of $w_i = \frac{1}{4}$. The 2D Pareto fronts and the corresponding volume fraction of the SRCs for an optimized replacement are presented.

bers. Prior to developing the optimization algorithm, the preliminary identification and selection of superior SRCs were based solely on relative comparisons of the F_i and r_{ij} values derived from the micromechanical model calibrated on the experimental data (Table D.3 and Table D.4, and Figure D.5). This oversimplified approach led to the initial selection of SRC3 and SRC0 for spring pads and tires, respectively. While the selection of a single SRC for individual properties may appear justified, it does not account for the lack of absolute superiority across all properties. As a consequence, choosing a single SRC to replace the entire volume fraction, v_T , is suboptimal in addressing the complex requirements of multi-property optimization. To overcome this limitation, our multi-objective optimization algorithm was developed and implemented to tackle the challenge of material selection. As demonstrated in Figure 4.4 to Figure 4.7, the algorithm generates Pareto fronts tailored to specific design scenarios, enabling the selection of optimal solutions based on combinations of objective functions and constraints. Each point on the Pareto front corresponds to a unique SRCs combination, providing a wider spectrum of potential solutions compared to the restrictive approach of selecting a single SRC. For instance, in the Pareto fronts for the spring pad application (Figure 4.4 and Figure 4.6(h)), although SRC3 emerges as a viable single choice for minimizing property deviations, however, depending on technical constraints or competitive market considerations, alternative points on the Pareto front may offer more advantageous trade-offs. Similarly, in the tire application (Figure 4.5 and Figure 4.7(f)), the comparison between selecting a single SRC such as SRC0 and exploring combinations along the Pareto front underscores the flexibility and adaptability of the proposed optimization framework. As a versatile alternative, the *Mean* point on these fronts, representing a balanced compromise across objective

functions, could be proposed as a robust and well-rounded selection. It demonstrates the versatility of the optimization algorithm in accommodating diverse design priorities and constraints, facilitating more informed and balanced decision-making in complex material selection problems.

In conclusion, this study introduces a versatile framework combining physically based machine learning and multi-objective optimization to optimize the integration of recycled materials with virgin resources. By balancing property deviations against economic and regulatory constraints, the framework demonstrates significant potential for advancing sustainable manufacturing practices, exemplified by its application in substituting raw rubber with recycled rubber in the automotive sector. The incorporation of a physics-informed machine learning approach enhances model precision, enabling accurate parameter calibration and effective handling of complex material behaviors. The framework's ability to manage multiple additives and property recoveries simultaneously underscores its flexibility and robustness, facilitating decision-making in material design. Validation against analytical solutions confirms the reliability of the proposed model, while its adaptability to diverse scenarios highlights its broad applicability. This work establishes a benchmark for sustainable material management, offering a scalable, cost-effective tool to reduce dependency on raw materials and promote recycling efficiency across various industries. This work directly addresses the challenges of circular economy and sustainable resource management by offering a scalable, data-driven approach that bridges material science, engineering, and sustainability policy. It supports the Sustainable Development Goals by promoting resource efficiency and reducing environmental impact, while providing a benchmark methodology applicable across industries.

Conclusion

Summary of Contributions

The key contributions can be summarized as follows:

- **Analytical Modeling of Lattices:** Classical Gibson–Ashby models were extended for 3D lattices (SC, BCC, BCC⁺) and 2D honeycombs, incorporating correction factors to account for functionally graded geometries and structural irregularities.
- **Dynamic Response Analysis:** Reduced-order, physics-informed models were developed to capture wave propagation and transient impact responses in graded lattice structures. The models successfully predict energy transmission, input/output accelerations, and attenuation characteristics.
- **Data-Driven and AI-Integrated Optimization:** A versatile framework combining micromechanical modeling, multi-objective optimization, and machine learning was developed to optimize the integration of recycled materials into virgin composites, balancing mechanical performance with economic and regulatory constraints.
- **Methodological Foundations:** Micromechanical methods (MOC, GMC, HFGMC) were explored to establish computational expertise and generate structured datasets, supporting the AI-driven and optimization studies in later chapters.

Synthesis of Findings

The research demonstrates that:

- Functionally graded and irregular lattice structures require correction factors in classical models to accurately predict their effective properties.
- Geometric parameters, irregularity, and mass distribution critically affect both static and dynamic responses of lattices, enabling tailored design for impact mitigation and energy absorption.

- Calibration factors were derived using Euler–Bernoulli beam assumptions for the 3D lattices in Chapter 1 and Timoshenko beams for the 2D lattices in Chapter 2, reflecting the dimensional tractability of each model and clarifying why κ (and η for irregularity) appear in different formulations.
- Physics-informed, data-driven frameworks can accelerate sustainable material design by efficiently combining simulations, experimental data, and optimization algorithms.
- For the truss-based lattices considered in this work, homogenized responses remain dominated by axial stiffness in the explored density ranges; bending and buckling effects stay negligible enough that higher-order (gradient or micropolar) continuum models do not emerge within the adopted homogenization assumptions.
- Dynamic analyses in Chapter III focus on time-domain responses and parametric variations; frequency-domain, modal, and resonance effects are not explicitly analyzed. Potential constructive/destructive wave interference phenomena due to lattice periodicity and grading are acknowledged but not explored, highlighting opportunities for deeper understanding of impact attenuation mechanisms.
- Analyses are performed by systematically varying design parameters (unit cell geometry, irregularity, and mass distribution) to interpret their influence on wave propagation and impact response, rather than applying explicit optimization.

Limitations

While the dissertation provides a comprehensive framework, several limitations remain:

- The analytical models only consider the elastic modulus relation with the relative density while the other properties such as Poisson’s ratio is not taken into consideration.
- Validation is limited to quasi-static uniaxial compression on a small number of samples; tensile, shear, bending, dynamic, and fatigue responses are not assessed.
- Only Vero polymers are considered; generalization to metals, elastomers, or other materials is not addressed.
- Number of experimental repetitions per configuration is small, limiting statistical reliability.

- κ/η charts are proposed as practical tools across wide ranges, but empirical checks cover only few geometries, one material, and one printing process.
- Some validation experiments fall in the higher relative density regime (0.29–0.68) where classical Gibson–Ashby models are less accurate; improved formulas for dense honeycombs are left for future work.
- Use of Euler–Bernoulli beams may introduce inaccuracies for stubby members or high-density lattices; boundary-layer, scale-dependence, and localization effects in graded lattices are not explicitly considered.
- Potential bending- or buckling-dominated regimes at extremely low relative densities are not explicitly analyzed; only axial-stiffness-dominated configurations are covered in the present homogenization framework.
- Homogenization is carried out using displacement-prescribed boundary conditions; alternative stress-prescribed schemes—which may yield different compliance estimates in heterogeneous media—are not explored here.
- In irregular honeycombs, only geometric perturbations are considered; possible variability in material elastic moduli is not included in the present formulation.
- Sensitivity analyses to quantify the effect of random fluctuations of material properties are not performed and remain outside the work’s current scope.
- Dynamic analyses focus on elastic behavior under impulsive loads; plasticity, fatigue, or viscoelastic effects are not explicitly addressed.
- The AI-driven framework, while versatile, depends on the quality and quantity of training data; generalization to entirely new material systems requires further validation.

Future Research Directions

Based on the findings and limitations, potential directions for future research include:

- Extending analytical and homogenization models to account for other mechanical properties and considering plasticity, viscoelasticity, and failure mechanisms.
- Expanding experimental validation to tension, shear, bending, dynamic, and fatigue tests, on a wider set of materials including metals and elastomers, with increased repetitions for better statistics.
- Developing improved analytical or numerical models for dense honeycombs and stubby beams (e.g., Timoshenko, second-gradient, or higher-order homogenization) and clarifying design rules for choosing κ , η , or model type based on density, member aspect ratio, and graded structure.

- Investigating boundary-layer effects, scale dependence, and localization in graded lattices, using full-scale simulations or localized experiments to validate homogenization assumptions.
- Extending the empirical validation of κ/η charts across broader geometries, materials, and manufacturing processes to confirm practical applicability.
- Extending Timoshenko-based formulations to 3D lattice geometries to assess shear effects, member stubby-ness, and potential improvements in κ/η calibration across a broader range of densities and architectures.
- Investigating lattice regimes in which beam bending, buckling, or second-gradient effects become significant, potentially requiring higher-order continuum representations.
- Exploring stress-prescribed homogenization strategies and comparing the resulting compliance estimates against displacement-prescribed results for highly heterogeneous and graded lattices.
- Perform systematic sensitivity studies to quantify the combined effects of geometric irregularity (f_1) and material property variations on the static and dynamic behavior of irregular honeycombs, including potential influence on homogenized properties and energy absorption.
- Investigating multidirectional grading (2D or 3D), re-entrant/auxetic lattice topologies, and TPMS structures, assessing their potential for enhanced energy absorption and novel applications.
- Expanding AI-driven frameworks to incorporate active learning, uncertainty quantification, and more diverse recycled material sources.
- Experimental validation of dynamic predictions and optimization frameworks for full-scale lattice and composite components.

Concluding Remarks

Overall, this dissertation provides an integrated approach to understanding, modeling, and optimizing architected materials and sustainable composites. By bridging analytical modeling, computational simulation, and data-driven optimization, it offers both theoretical insights and practical tools for engineering design. The findings contribute to advancing lightweight, high-performance, and environmentally responsible material solutions in diverse applications.

Appendices

APPENDIX A

A Modified Gibson-Ashby Model for Functionally Graded Lattice Structures

A.1 Calculation of the relative density of k th cell

Consider the k th cell in a graded lattice that has three types of ligaments. The dimensionless diameter, R , of the first type of ligaments located on the $(k-1)$ th and k th $y-z$ planes are defined in Equation (1.2) and the dimensionless diameter of the second type ligaments which are parallel to x axis varies linearly from $R_{yz}^{(k-1)}$ to $R_{yz}^{(k)}$ forming four tapered ligaments. The dimensionless diameter of the third type, i.e., diagonal ligaments, is the average of $R_{yz}^{(k-1)}$ and $R_{yz}^{(k)}$ as explained in Equation (1.3). To find the relative density, first, the ratio of the volume of a single ligament, V_{lig} to the volume of the cell, V_0 is needed for all three types. Note that the first and the third types have a cylindrical shape while the second type is a conical frustum. The volume ratio of a cylindrical ligament is:

$$\left(\frac{V_{lig}}{V_0} \right)_{cylinder} = \frac{(\pi/4)d^2\hat{l}}{l^3} \quad (A.1)$$

while for a tapered ligament with the ending diameters d_1 and d_2 it is:

$$\left(\frac{V_{lig}}{V_0} \right)_{taper} = \frac{(\pi/12)(d_1^2 + d_1d_2 + d_2^2)\hat{l}}{l^3} \quad (A.2)$$

where $\hat{l} = l$ or $\hat{l} = \sqrt{3}l$ is the length of the ligament on the sides or on diagonals, respectively. Applying the dimensionless diameter definition, $R = d/l$, the dimensionless form of the volume ratios of the ligaments constructing k th unit cell are obtained:

$$\left(\frac{V_{lig}}{V_0}\right)_{yz}^{(k-1)} = \frac{\pi}{4} \left(R_{yz}^{(k-1)}\right)^2 \quad (\text{A.3a})$$

$$\left(\frac{V_{lig}}{V_0}\right)_{yz}^{(k)} = \frac{\pi}{4} \left(R_{yz}^{(k)}\right)^2 \quad (\text{A.3b})$$

$$\left(\frac{V_{lig}}{V_0}\right)_{diagonal}^{(k)} = \frac{\pi\sqrt{3}}{4} \left(R_{ave}^{(k)}\right)^2 \quad (\text{A.3c})$$

$$\left(\frac{V_{lig}}{V_0}\right)_x^{(k)} = \frac{\pi}{12} \left[\left(R_{yz}^{(k-1)}\right)^2 + R_{yz}^{(k-1)} R_{yz}^{(k)} + \left(R_{yz}^{(k)}\right)^2 \right] \quad (\text{A.3d})$$

Then, the relative density of the unit cell is given by summation over the volume ratio of all ligaments noticing that the ligaments on the sides are shared with the four adjacent cells while the diagonal ligaments exclusively belong to the cell. For SC, BCC, and BCC⁺ lattices, it yields:

$$\left(\frac{\rho}{\rho_0}\right)_{SC}^{(k)} = \frac{4}{4} \left[\left(\frac{V_{lig}}{V_0}\right)_{yz}^{(k-1)} + \left(\frac{V_{lig}}{V_0}\right)_{yz}^{(k)} + \left(\frac{V_{lig}}{V_0}\right)_x^{(k)} \right] \quad (\text{A.4a})$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC}^{(k)} = 4 \left(\frac{V_{lig}}{V_0}\right)_{diagonal}^{(k)} \quad (\text{A.4b})$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC^+}^{(k)} = \left(\frac{\rho}{\rho_0}\right)_{SC}^{(k)} + \left(\frac{\rho}{\rho_0}\right)_{BCC}^{(k)} \quad (\text{A.4c})$$

Substituting Equation (A.3), Equation (1.2), and Equation (1.3) into Equation (A.4) and some simplifications give the expression for relative density of k th cell of the graded SC, BC, and BCC⁺ lattices:

$$\left(\frac{\rho}{\rho_0}\right)_{SC}^{(k)} = \left[a_1^{(k)} R_0^2 + a_2^{(k)} (\Delta R)(R_0) + a_3^{(k)} \Delta R^2 \right] \quad (\text{A.5a})$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC}^{(k)} = \left[a_4^{(k)} R_0^2 + a_5^{(k)} (\Delta R)(R_0) + a_6^{(k)} \Delta R^2 \right] \quad (\text{A.5b})$$

$$\left(\frac{\rho}{\rho_0}\right)_{BCC^+}^{(k)} = \left[a_7^{(k)} R_0^2 + a_8^{(k)} (\Delta R)(R_0) + a_9^{(k)} \Delta R^2 \right] \quad (\text{A.5c})$$

where the coefficients $a_i^{(k)}$ are:

$$a_1^{(k)} = 3\pi/4 \quad (\text{A.6a})$$

$$a_2^{(k)} = a_1^{(k)} \frac{(k-1)^m + k^m}{N^m} \quad (\text{A.6b})$$

$$a_3^{(k)} = a_1^{(k)} \frac{4(k-1)^{2m} + 4k^{2m} + k^m(k-1)^m}{9N^{2m}} \quad (\text{A.6c})$$

$$a_4^{(k)} = \pi\sqrt{3} \quad (\text{A.6d})$$

$$a_5^{(k)} = a_4^{(k)} \frac{(k-1)^m + k^m}{N^m} \quad (\text{A.6e})$$

$$a_6^{(k)} = a_4^{(k)} \frac{((k-1)^m + k^m)^2}{4N^{2m}} \quad (\text{A.6f})$$

$$a_7^{(k)} = a_1^{(k)} + a_4^{(k)} \quad (\text{A.6g})$$

$$a_8^{(k)} = a_2^{(k)} + a_5^{(k)} \quad (\text{A.6h})$$

$$a_9^{(k)} = a_3^{(k)} + a_6^{(k)} \quad (\text{A.6i})$$

A.2 Calculation of the relative elastic modulus of k th cell

Here, the detailed calculations of relative elastic modulus for the k th cell of SC, BCC, and BCC⁺ graded lattices based on Euler-Bernoulli beam theory are presented. The elongation of a bulk unit cell, δ_0 with the elastic modulus E_0 and the area $A_0 = l^2$ under an applied force, P , is:

$$\delta_0 = \frac{P}{lE_0} \quad (\text{A.7})$$

Given the elongation of the lattice unit cell, δ under the same load, the relative elastic modulus of the cell is obtained, as shown in Figure A.1:

$$\frac{E}{E_0} = \frac{\delta_0}{\delta} = \frac{P}{lE_0\delta} \quad (\text{A.8})$$

SC graded lattice: In an SC unit cell, the ligaments on $y-z$ planes are not contributing when the load is applied along the x axis and the load is carried out by the four tapered ligaments parallel to x . For a tapered bar with the length $\hat{L}_1$ and the diameters of d_1 and d_2 under an applied axial load, f_t , the variable cross-section area, $A(x)$ and then the elongation, δ_{taper} , are:

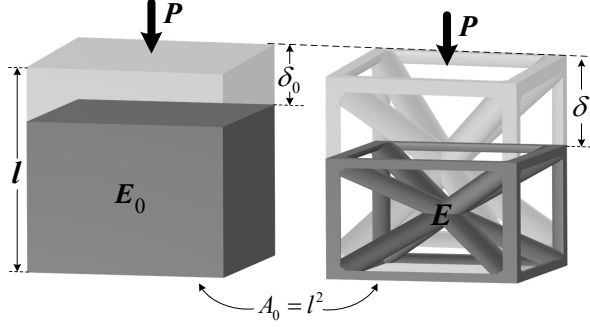


Figure A.1. The schematic of comparison between the elongation of the bulk and the unit cell of graded lattice for finding the relative modulus by Equation (A.8).

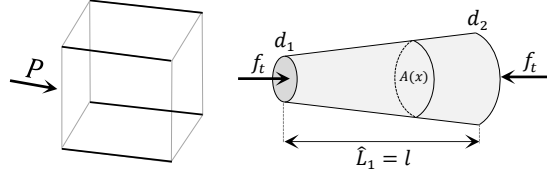


Figure A.2. The tapered representative beam for calculating the relative density of the graded SC lattice.

$$A(x) = \frac{\pi}{4} \left(d_1 - (d_1 - d_2) \left(\frac{x}{\hat{L}_1} \right) \right)^2 \quad (\text{A.9a})$$

$$\delta_{taper} = \frac{f_t}{E_0} \int_0^{\hat{L}_1} \frac{1}{A(x)} dx = \frac{4f_t \hat{L}_1}{\pi E_0 d_1 d_2} \quad (\text{A.9b})$$

Note that each of these ligaments is shared with four adjacent cells, and it means that every unit cell enjoys the benefit of one full tapered ligament in total, as shown in Figure A.2. Hence, elongation of the SC unit cell with tapered lattice, δ_{SC} , is obtained by Setting $\hat{L}_1 = l$, and $f_t = P$ in Equation (A.9b):

$$\delta_{SC} = \frac{4Pl}{\pi E_0 d_1 d_2} \quad (\text{A.10})$$

Substituting Equation (A.10) into Equation (A.8) yields the relative density of the SC unit cell with tapered ligaments:

$$\left(\frac{E}{E_0} \right)_{SC, taper} = \frac{\pi}{4} \frac{d_1}{l} \frac{d_2}{l} \quad (\text{A.11})$$

For the k th unit cell of the SC graded lattice, the diameter to length ratios in Equation (A.11) are replaced with $R_{yz}^{(k-1)}$ and $R_{yz}^{(k)}$ resulting in:

$$\left(\frac{E}{E_0}\right)_{SC}^{(k)} = \frac{\pi}{4} R_{yz}^{(k-1)} R_{yz}^{(k)} \quad (\text{A.12})$$

which is simplified to

$$\left(\frac{E}{E_0}\right)_{SC}^{(0)} = \frac{\pi}{4} R^2 \quad (\text{A.13})$$

for a uniform SC lattice with identical ligaments' diameters.

BCC graded lattice: Taking the advantage of symmetry, only one-eighth of the unit cell, i.e., a single inclined ligament of length $\hat{L}_2 = \sqrt{3}(l/2)$ carrying a quarter of unit cell load, $P/4$, is considered in the analytical solution to find the elongation of the BCC unit cell (see Figure A.3). Since the joints are assumed to be rigid, the slopes of the ligament at both ends are zero. The applied load, P is decomposed to its components, f_η and f_ζ , along the local axial, η , and transverse, ζ coordinate of the ligament:

$$f_\eta = \frac{\sqrt{3}}{3} P \quad (\text{A.14a})$$

$$f_\zeta = \frac{\sqrt{2}}{\sqrt{3}} P \quad (\text{A.14b})$$

To keep the slope zero, an additional moment, $M_z = f_\zeta \hat{L}_2/2$, is applied from the rigid joint. It results in an axial, u_η , and a transverse, u_ζ , displacement at the free tip of the ligament:

$$u_\eta = \frac{f_\eta \hat{L}_2}{AE_0} \quad (\text{A.15a})$$

$$u_\zeta = \frac{f_\zeta \hat{L}_2^3}{12E_0 I} \quad (\text{A.15b})$$

where $A = (\pi/4)d^2$ and $I = (\pi/64)d^4$ for the circular cross-section. Then, the displacement of the ligament tip along the load P , i.e., x axis, is calculated as:

$$u_x = \frac{\sqrt{3}}{3} u_\eta + \frac{\sqrt{2}}{\sqrt{3}} u_\zeta \quad (\text{A.16})$$

Substituting Equation (A.15), Equation (A.14), into Equation (A.16) gives the total elongation of the BCC unit cell, δ_{BCC} as the twice of u_x :

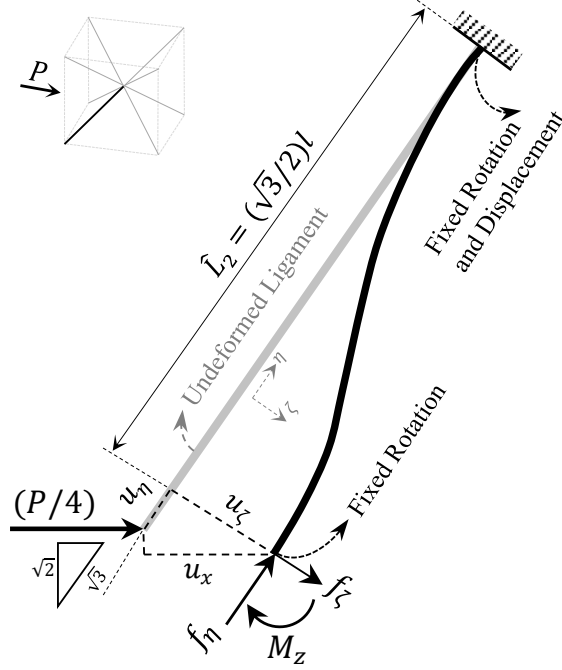


Figure A.3. The Euler-Bernoulli beam model for calculating the relative density of the graded BCC lattice.

$$\delta_{BCC} = 2u_x = \frac{P}{\sqrt{3}\pi E_0} \left(\frac{l}{d^2} + 2\frac{l^3}{d^4} \right) \quad (\text{A.17})$$

Substituting Equation (A.17) into Equation (A.8) yields the relative elastic modulus:

$$\left(\frac{E}{E_0} \right)_{BCC}^{(0)} = \pi\sqrt{3} \left(\frac{R^4}{2 + R^2} \right) \quad (\text{A.18})$$

The relative elastic modulus of k th unit cell of the BCC lattice is simply given by replacing R with $R_{ave}^{(k)}$ since it is assumed that the diagonal ligaments are cylindrical:

$$\left(\frac{E}{E_0} \right)_{BCC}^{(k)} = \pi\sqrt{3} \left(\frac{(R_{ave}^{(k)})^4}{2 + (R_{ave}^{(k)})^2} \right) \quad (\text{A.19})$$

BCC⁺ graded lattice: The representative frame of the BCC⁺ lattice for the analytical calculation consists of four inclined ligaments of length $\hat{L}_2 = (\sqrt{3}/2)l$, the diameter

d_3 , a tapered ligament with length $\hat{L}_1 = (l/2)$ and ending diameters d_1 and d_2 . The connecting joint moves only along the x axis because of the symmetry of the inclined ligaments and the fact that the tapered one must remain straight. The schematic of this representative frame is displayed in Figure A.4, while for better visibility only one of four inclined ligaments is depicted.

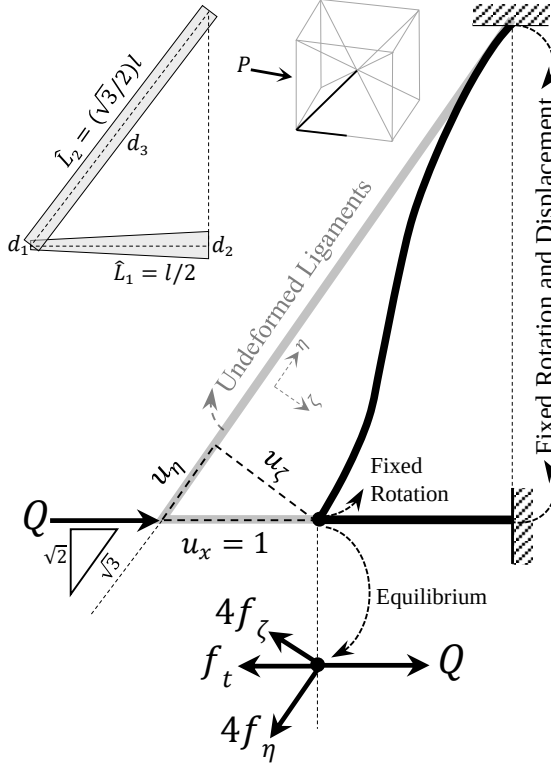


Figure A.4. The Euler-Bernoulli beam model for calculating the relative density of the graded BCC⁺ lattice.

Here, a unity displacement, $u_x = 1$ is applied to the connecting joint and the equivalent required the corresponding load, Q is evaluated from the equilibrium which is equal to the effective stiffness of the frame, K_{eq} :

$$Q = K_{eq}u_x = K_{eq} \quad (\text{A.20})$$

The applied unity displacement causes a unity elongation of tapered ligament and a reaction force, f_t , along the x axis. This reaction force is obtained from Equation (A.9b) by setting $\delta_{taper} = 1$ and solving for f_t :

$$f_t = \frac{\pi E_0 d_1 d_2}{4 \hat{L}_1} \quad (\text{A.21})$$

Besides, it imposes an axial displacement, $u_\eta = (\sqrt{3}/3)$, and a transverse displacement, $u_\zeta = (\sqrt{2}/\sqrt{3})$ to each inclined ligament. Replacing these values to Equation (A.15) and solving for f_η and f_ζ , gives the reaction forces of each inclined ligament on the joint:

$$f_\eta = \frac{\sqrt{3}}{3} \frac{AE_0}{\hat{L}_2} \quad (\text{A.22a})$$

$$f_\zeta = \frac{\sqrt{2}}{\sqrt{3}} \frac{12E_0 I}{\hat{L}_2^3} \quad (\text{A.22b})$$

The equilibrium along the x axis gives the force Q which results in the assumed unity displacement:

$$Q = f_t + 4 \frac{\sqrt{3}}{3} f_\eta + 4 \frac{\sqrt{2}}{\sqrt{3}} f_\zeta \quad (\text{A.23})$$

Substituting Equation (A.21), Equation (A.22), and Equation (A.20) into Equation (A.23) and setting $\hat{L}_1 = l/2$, $\hat{L}_2 = (\sqrt{3}/2)l$, $A = (\pi/4)d_3^2$, and $I = (\pi/64)d_3^4$, yields the equivalent stiffness of the frame:

$$K_{eq} = \frac{\pi l E_0}{2} \left(\frac{d_1}{l} \frac{d_2}{l} + \frac{4\sqrt{3}}{9} \left(\left(\frac{d_3}{l} \right)^2 + 2 \left(\frac{d_3}{l} \right)^4 \right) \right) \quad (\text{A.24})$$

The k th unit cell of the BCC^+ lattice can be assumed as a combination of two frames, I and II, assembled in series. In the frame I, the dimensionless diameters are $R_1 = (d_1/l) = R_{yz}^{(k-1)}$, $R_2 = (d_2/l) = R_{ave}^{(k)}$, and $R_3 = (d_3/l) = R_{ave}^{(k)}$, while for the frame II, they are $R_1 = (d_1/l) = R_{ave}^{(k)}$, $R_2 = (d_2/l) = R_{ave}^{(k)}$, and $R_3 = R_{yz}^{(k1)}$ (see Figure A.5). Replacing these dimensionless diameters in Equation (A.24), the effective stiffness of these two frames is calculated as:

$$(K_{eq})_I = \frac{\pi l E_0}{2} \left(R_{yz}^{(k-1)} R_{ave}^{(k)} + \frac{4\sqrt{3}}{9} \left(\left(R_{ave}^{(k)} \right)^2 + 2 \left(R_{ave}^{(k)} \right)^4 \right) \right) \quad (\text{A.25a})$$

$$(K_{eq})_{II} = \frac{\pi l E_0}{2} \left(R_{ave}^{(k)} R_{yz}^{(k)} + \frac{4\sqrt{3}}{9} \left(\left(R_{ave}^{(k)} \right)^2 + 2 \left(R_{ave}^{(k)} \right)^4 \right) \right) \quad (\text{A.25b})$$

and the total effective stiffness of the unit cell, $(K_{eq})_{\text{BCC}^+}$, is the combination of these two springs in series:

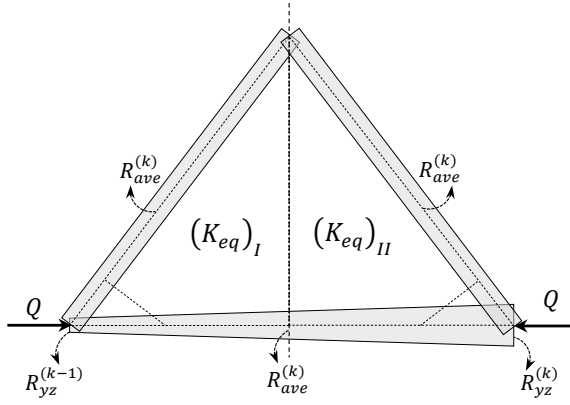


Figure A.5. The Euler-Bernoulli beam model for calculating the relative density of the graded BCC⁺ lattice.

$$(K_{eq})_{BCC^+} = \frac{(K_{eq})_I (K_{eq})_{II}}{(K_{eq})_I + (K_{eq})_{II}} \quad (\text{A.26})$$

Having the total stiffness of the unit cell, its elongation due to the applied load P is obtained as:

$$\delta_{BCC^+} = \frac{P}{(K_{eq})_{BCC^+}} \quad (\text{A.27})$$

Then, replacing this elongation in Equation (A.8) yields the relative stiffness of the BCC⁺ unit cell:

$$\left(\frac{E}{E_0} \right)_{BCC^+} = \frac{b_1^{(k)} b_2^{(k)}}{b_1^{(k)} + b_2^{(k)}} \quad (\text{A.28})$$

where

$$b_1^{(k)} = \frac{\pi}{2} \left(R_{yz}^{(k-1)} R_{ave}^{(k)} + \frac{4\sqrt{3}}{9} \left((R_{ave}^{(k)})^2 + 2 (R_{ave}^{(k)})^4 \right) \right) \quad (\text{A.29a})$$

$$b_2^{(k)} = \frac{\pi}{2} \left(R_{ave}^{(k)} R_{yz}^{(k)} + \frac{4\sqrt{3}}{9} \left((R_{ave}^{(k)})^2 + 2 (R_{ave}^{(k)})^4 \right) \right) \quad (\text{A.29b})$$

For the special case of uniform BCC⁺ unit cell with the ligaments of identical dimensionless diameter, R , the coefficients $b_1^{(k)}$ and $b_2^{(k)}$ are equal and independent from k and the relative elastic modulus simplifies to:

$$\left(\frac{E}{E_0}\right)_{BCC^+}^{(0)} = \frac{\pi}{4} \left(\left(1 + \frac{4\sqrt{3}}{9}\right) R^2 + \frac{8\sqrt{3}}{9} R^4 \right) \quad (A.30)$$

A.3 Curve fitting parameters α and β for the equivalent density and modulus

Figure A.6 and Figure A.7, illustrate the curve fitting parameters α and β defined in Equation (1.9) for the continuous functions of relative density and relative modulus for SC, BCC, and BCC⁺ graded lattices. Graphs are presented for a wide range of dimensionless diameter combinations, i.e., $R_0 = 0.05, 0.07, 0.1, 0.12, 0.14, 0.17, 0.21, 0.25$, and 0.3 , and for each $R_0 < R_N < 0.5$. The presented α and β parameters are obtained by the best fitting of Equation (1.9) to Equation (1.6) and Equation (1.7) for a high-resolution graded lattice with $N = 100$ implementing the least square approach. For intermediate values of R_0 which are not presented in Figure A.6 and Figure A.7 one can obtain the α and β parameters via interpolation or use the following simplified approximation:

$$\begin{aligned} \alpha, \beta = & A_1 R_0 + A_2 R_0^2 + A_3 R_0^3 + A_4 R_0^4 + A_5 R_0^5 \\ & + B_1 R_N + B_2 R_N^2 + B_3 R_N^3 + B_4 R_N^4 + B_5 R_N^5 \\ & + C_1 R_0^4 R_N + C_2 R_0^3 R_N^2 + C_3 R_0^2 R_N^3 + C_4 R_0 R_N^4 \\ & + C_5 R_0^3 R_N + C_6 R_0^2 R_N^2 + C_7 R_0 R_N^3 \\ & + C_8 R_0^2 R_N + C_9 R_0 R_N^2 \\ & + C_{10} R_0 R_N + D \end{aligned} \quad (A.31)$$

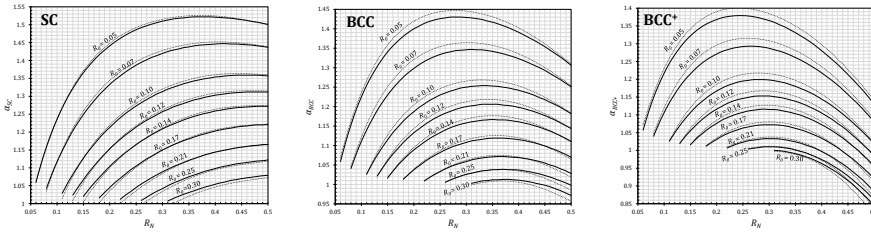
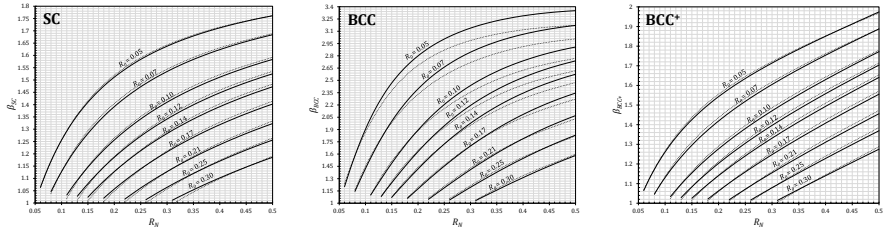


Figure A.6. The curve fitting parameter α for SC, BCC, and BCC⁺. Dashed lines are from Equation (A.31)

	α_{SC}	α_{BCC}	α_{BCC^+}	β_{SC}	β_{BCC}	β_{BCC^+}
A_1	-12.100	-11.880	-11.850	-12.480	-40.910	-12.480
A_2	59.660	59.110	58.220	61.040	197.800	60.670
A_3	-114.200	-111.700	-103.400	-117.300	-174.400	-118.200
A_4	93.460	89.070	62.650	91.530	-114.100	92.800
A_5	-27.070	-24.390	6.417	-23.810	72.050	-23.580
B_1	9.306	9.081	8.769	9.688	31.900	9.687
B_2	-46.610	-46.850	-46.400	-45.510	-154.900	-44.540
B_3	116.500	115.900	114.400	112.800	356.300	113.000
B_4	-150.800	-149.800	-148.600	-144.300	-400.200	-145.300
B_5	78.840	77.760	76.540	75.020	176.700	75.580
C_1	-97.510	-90.840	-96.230	-103.600	13.600	-106.700
C_2	-130.300	-137.900	-145.300	-142.100	-983.100	-139.900
C_3	-49.620	-47.240	-70.660	-32.120	-417.100	-30.700
C_4	87.770	84.870	69.200	89.350	706.500	87.930
C_5	229.100	229.400	239.800	245.900	946.500	247.300
C_6	147.100	148.000	168.000	134.000	1177.000	130.100
C_7	-122.100	-120.300	-96.850	-131.300	-980.900	-129.000
C_8	-151.600	-151.900	-159.000	-153.000	-884.000	-151.200
C_9	44.490	43.130	29.820	53.120	362.200	52.020
C_{10}	12.550	13.280	16.660	9.983	40.650	9.386
D	1.090	1.104	1.116	1.090	1.324	1.095

Table A.1. The dimensionless constants for Equation (A.31)**Figure A.7.** The curve fitting parameter β for SC, BCC, and BCC⁺. Dashed lines are from Equation (A.31)

A.4 Graphical presentation of effective modulus and effective density of graded lattices

Figure A.8 to Figure A.13, depict the relative effective density and the relative effective elastic modulus of fully homogenized SC, BCC, and BCC⁺ graded lattices according to the exact series expressions in Equation (1.10) and Equation (1.15). Graphs are presented for three different powers for grading, $m = 1, 2$, and 3 , and a wide range of dimensionless diameter combinations, i.e., $R_0 = 0.05, 0.1, 0.15, 0.2, 0.25$, and 0.3 , and for each $R_0 < R_N < 0.5$, which can be used as a design guide for tuning the effective properties of the graded lattice.

A.5 The calibrated correction factor κ for the modified Gibson-Ashby model

Figure A.14 depicts the calibrated correction factor, κ in Equation (1.21), for the proposed modified Gibson-Ashby model relating the effective relative elastic modulus to the effective relative density of SC, BCC, and BCC⁺ graded lattices, Equation (1.20), and its local form, Equation (1.23). Graphs are plotted for three different power of grading, $m = 1, 2$, and 3 , and a wide range of the ratio, $1 < (R_N/R_0) < 5$ considering a high resolution of $N = 100$. Note that for all the plots, the value of κ starts from one where $(R_N/R_0) = 1$ corresponds to a uniform lattice (standard Gibson-Ashby model in Equation (2.15)).

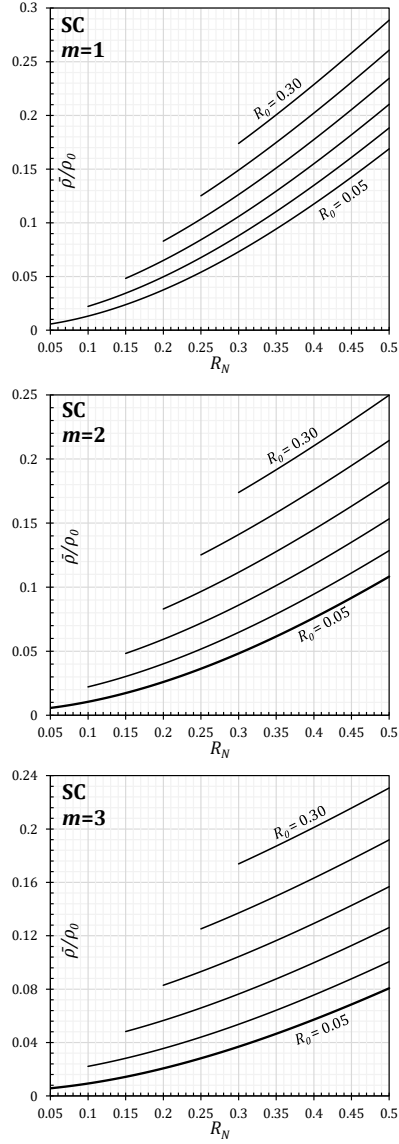


Figure A.8. The relative effective density of SC lattices for the power $m = 1, 2$, and 3 , and different values of R_0 and R_N .

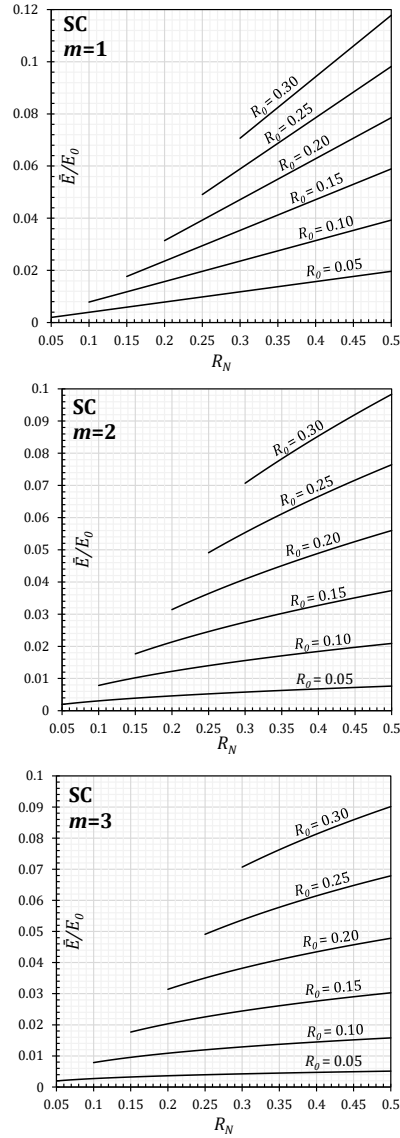


Figure A.9. The relative effective elastic modulus of SC lattices for the power $m = 1, 2$, and 3, and different values of R_0 and R_N .

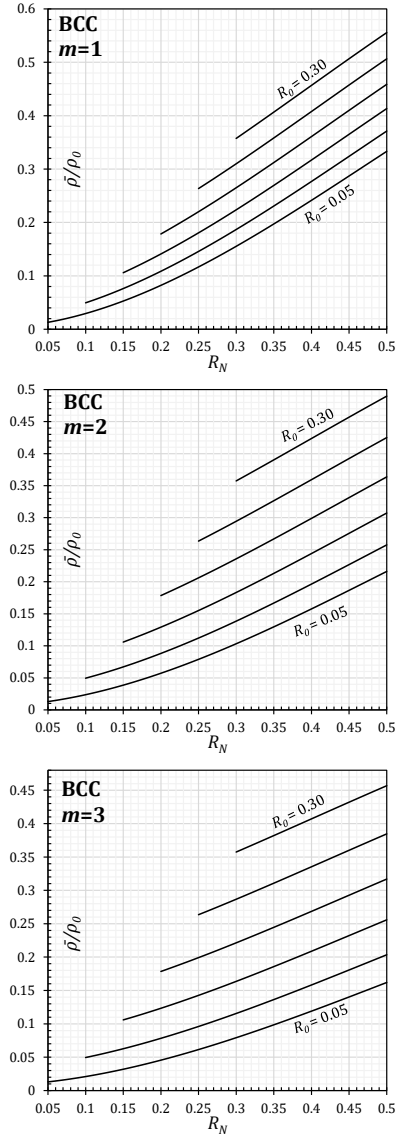


Figure A.10. The relative effective density of BCC lattices for the power $m = 1, 2$, and 3 , and different values of R_0 and R_N .

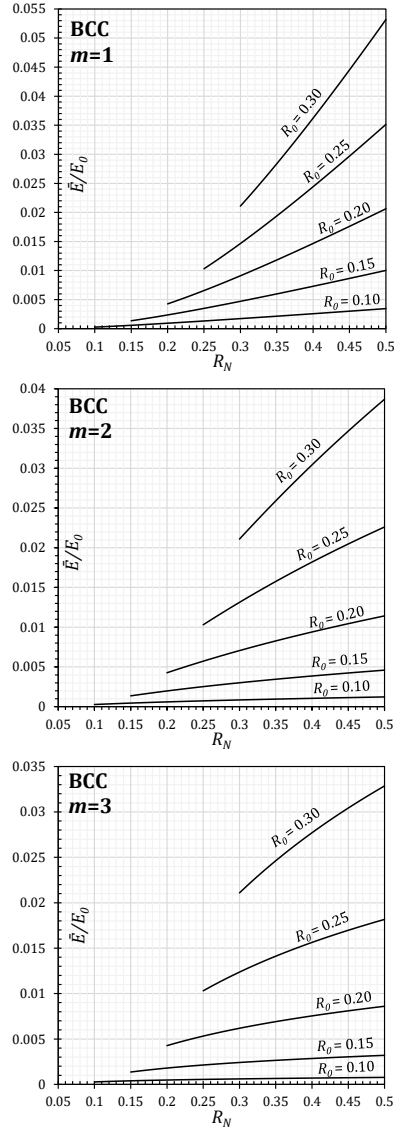


Figure A.11. The relative effective elastic modulus of BCC lattices for the power $m = 1$, 2, and 3, and different values of R_0 and R_N .

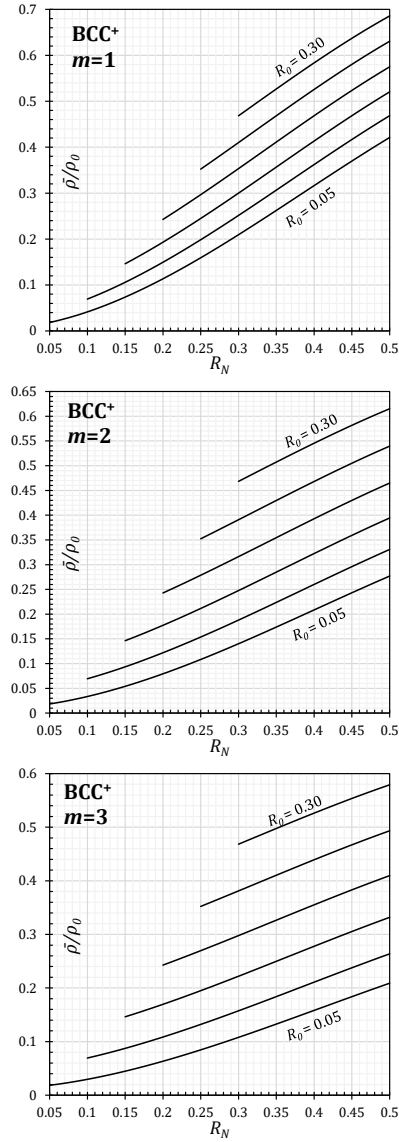


Figure A.12. The relative effective density of BCC⁺ lattices for the power $m = 1, 2$, and 3 , and different values of R_0 and R_N .

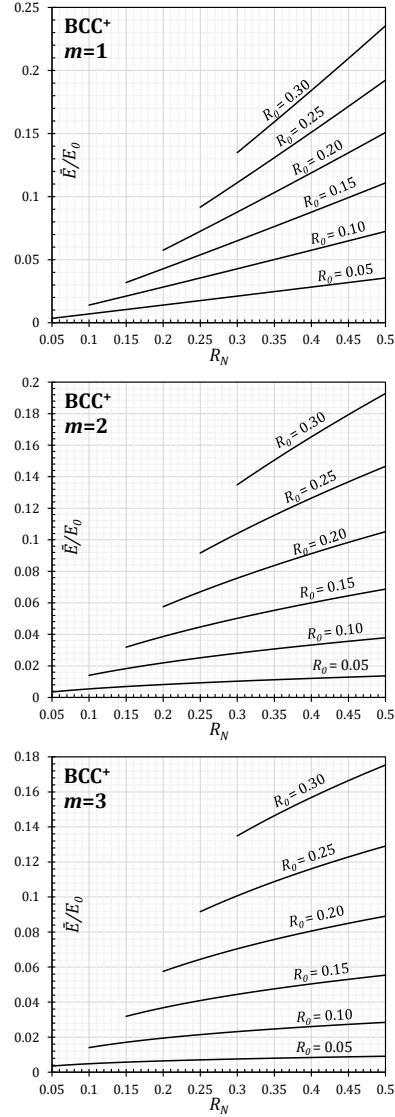


Figure A.13. The relative effective elastic modulus of BCC⁺ lattices for the power $m = 1, 2$, and 3 , and different values of R_0 and R_N .

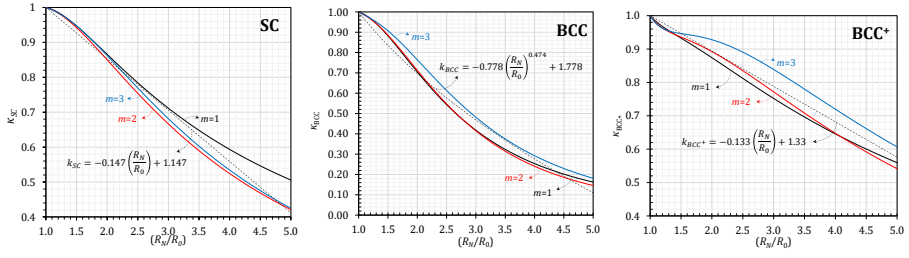


Figure A.14. The calibrated κ parameter versus (R_N/R_0) for SC, BCC, and BCC⁺ graded lattices and the power $m = 1, 2$, and 3.

APPENDIX B

A Refined Gibson-Ashby Model for Functionally Graded Honeycombs with Random Irregularities

B.1 Supplementary Figures

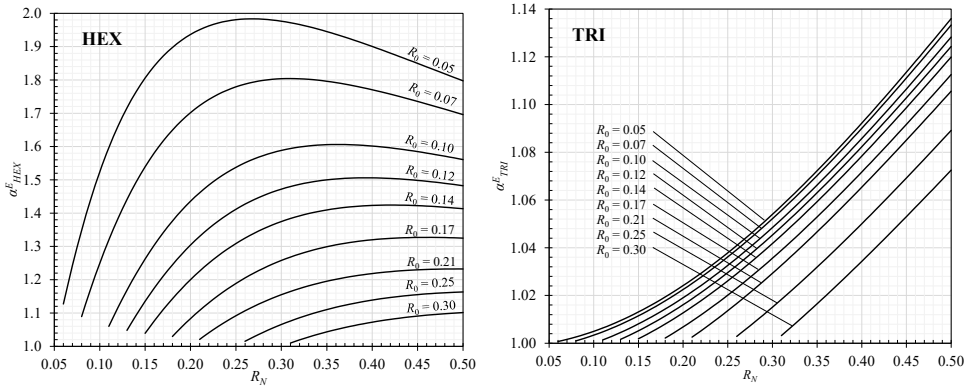


Figure B.1. The curve fitting parameter α for the relative elastic modulus of the honeycomb structure with HEX and TRI unit cell.

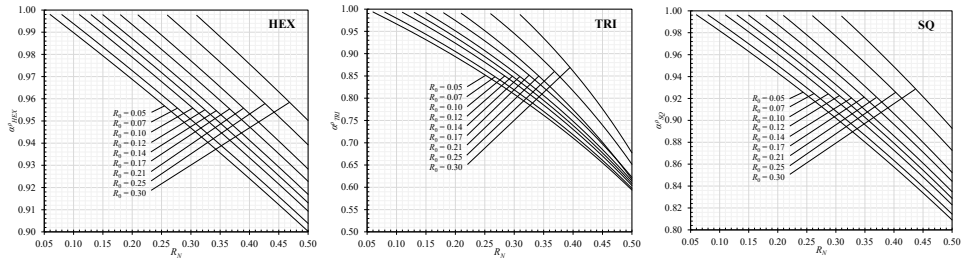


Figure B.2. The curve fitting parameter α for relative density of the honeycomb structure with HEX, TRI, and SQ unit cell.

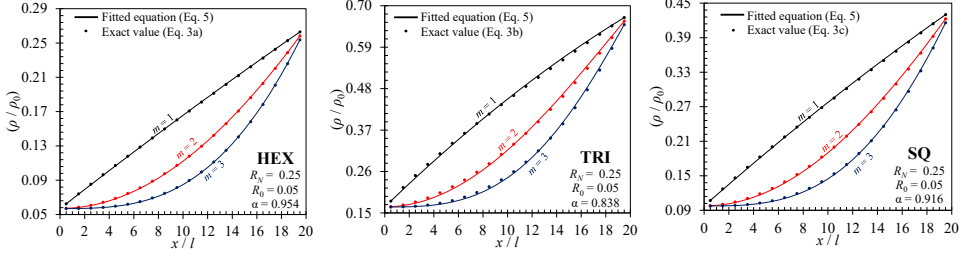


Figure B.3. Comparison of the results of the continuous formulation for relative density (Equation (2.7)) with the exact solution (Equation (2.5)).

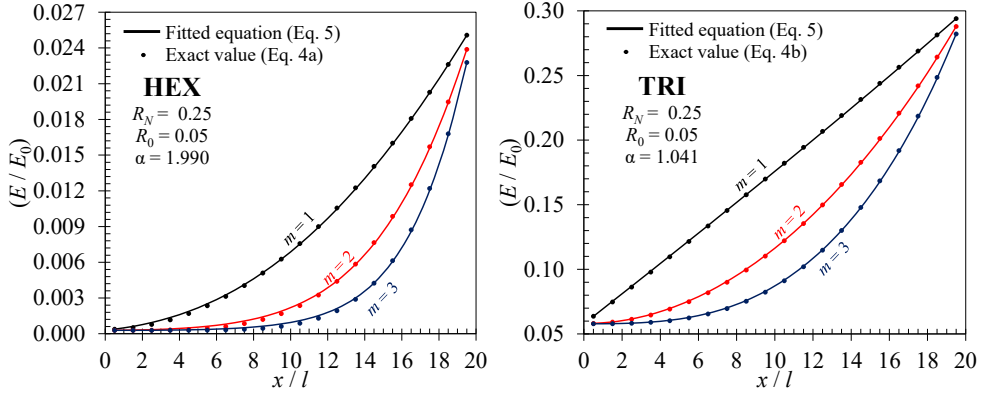


Figure B.4. Comparison of the results of the continuous formulation for relative elastic modulus (Equation (2.7)) with the exact solution (Equation (2.6)).

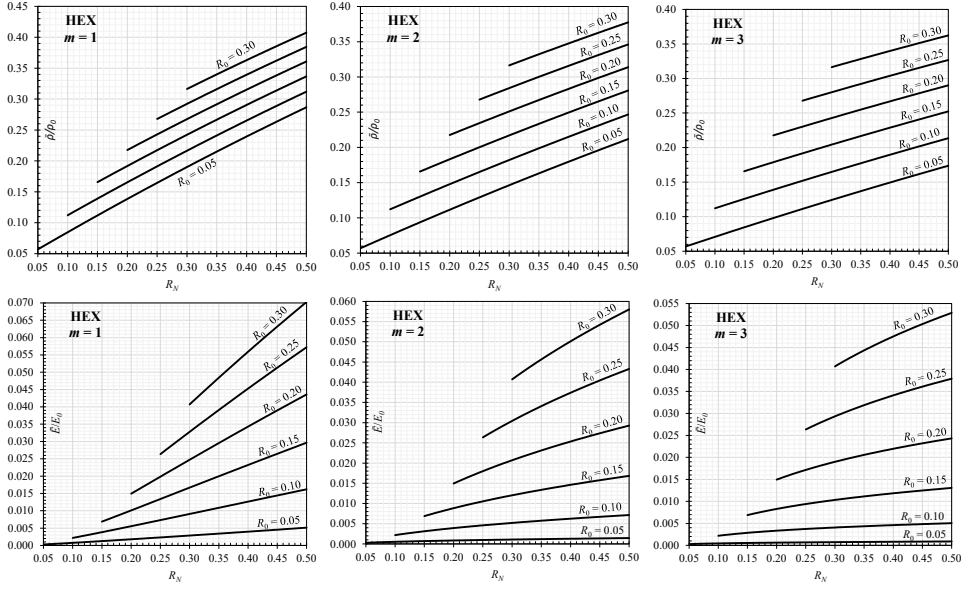


Figure B.5. Effective relative density and effective elastic modulus for FG honeycombs with HEX unit cell.

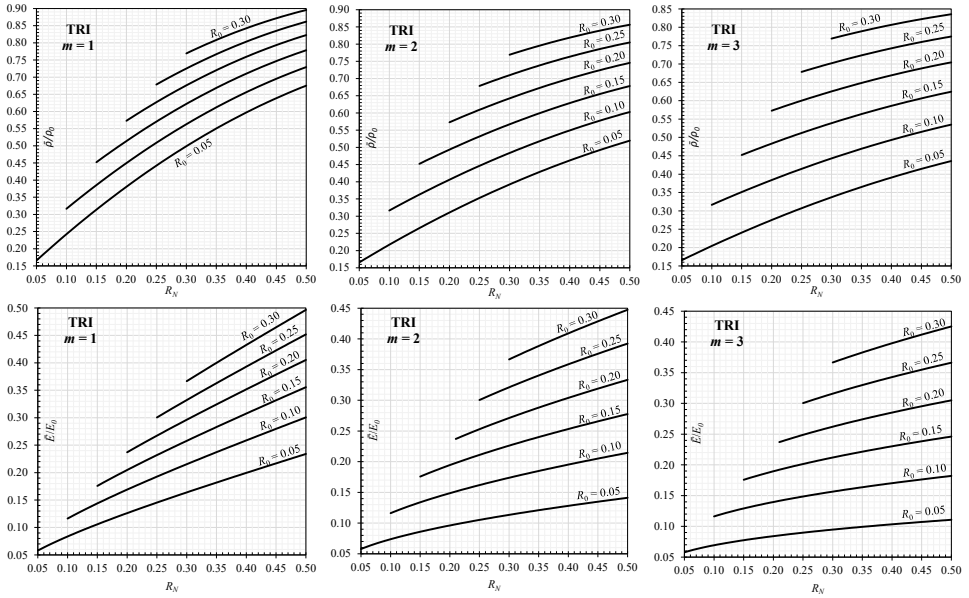


Figure B.6. Effective relative density and effective elastic modulus for FG honeycombs with TRI unit cell.

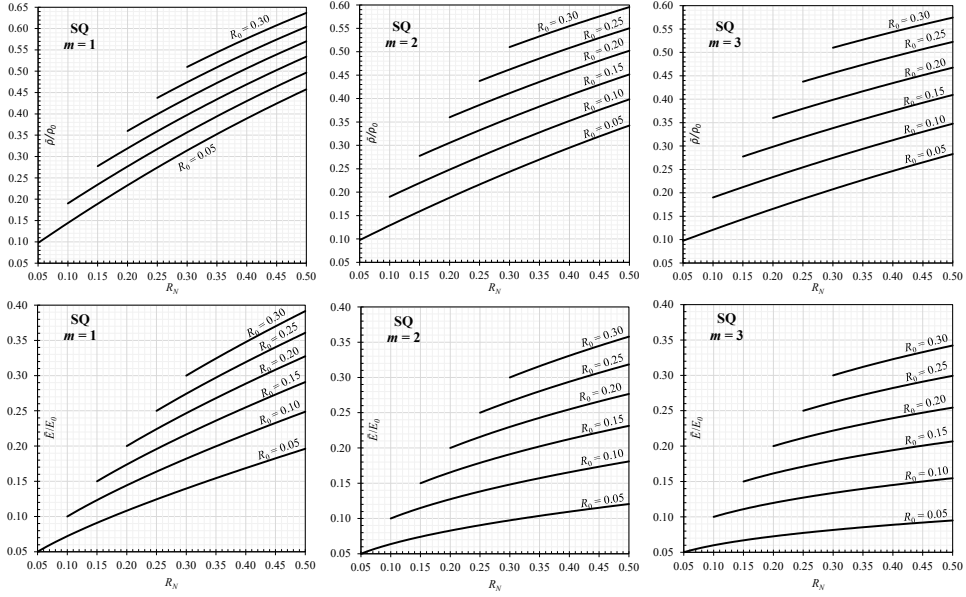


Figure B.7. Effective relative density and effective elastic modulus for FG honeycombs with SQ unit cell.

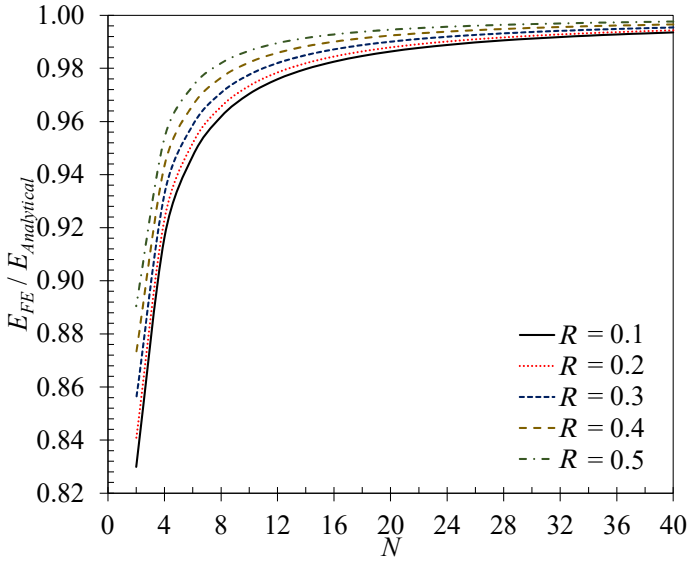


Figure B.8. Effect of unit cell number on the elastic modulus obtained by the FE model compared to the analytical one for the uniform honeycombs with TRI unit cell and for different aspect ratios, R .

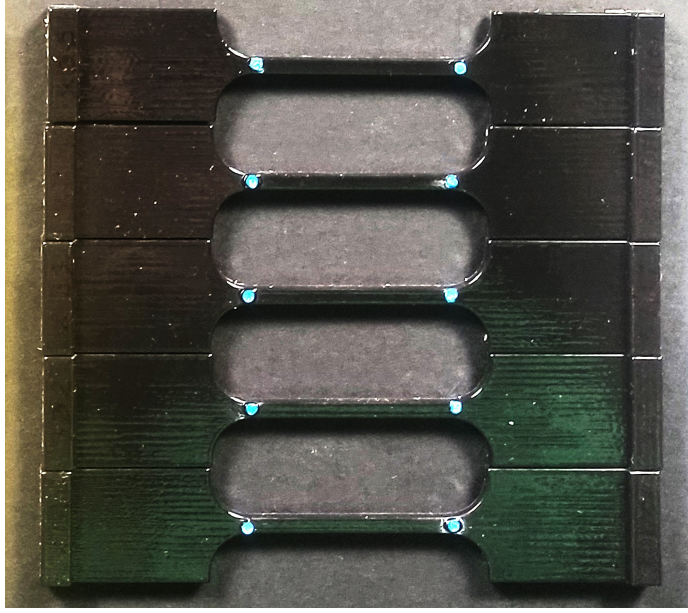


Figure B.9. The manufactured dog-bone specimens underwent uniaxial testing to assess the elastic modulus of the bulk material (Vero PureBlack™), which was employed for printing the FG honeycombs.

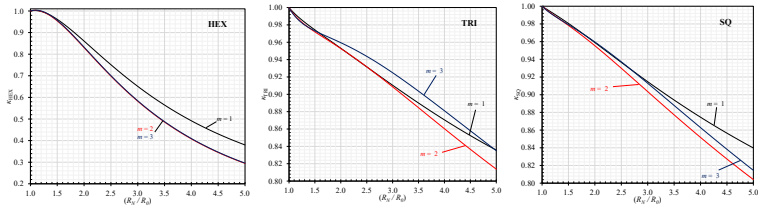


Figure B.10. The calibrated parameter κ for the honeycomb structure with HEX, TRI, and SQ unit cell.

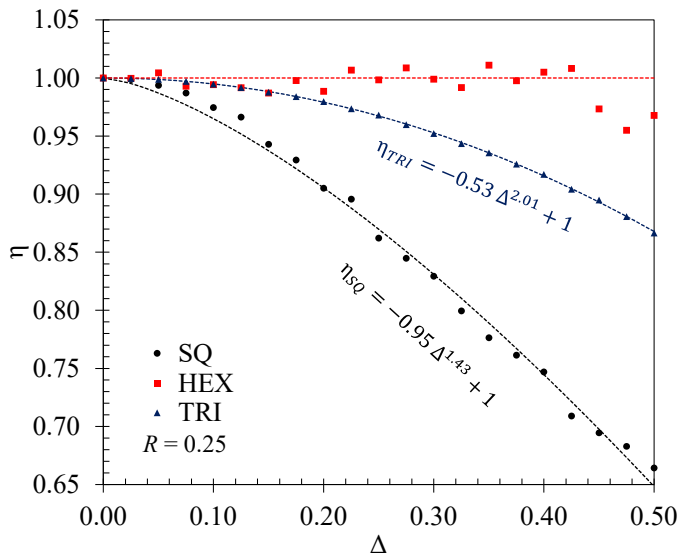
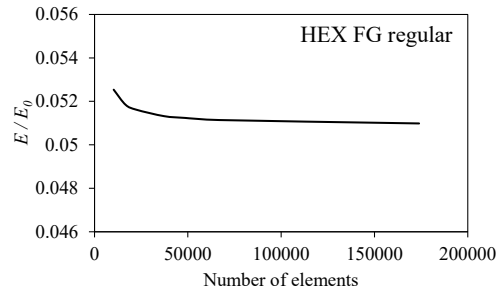
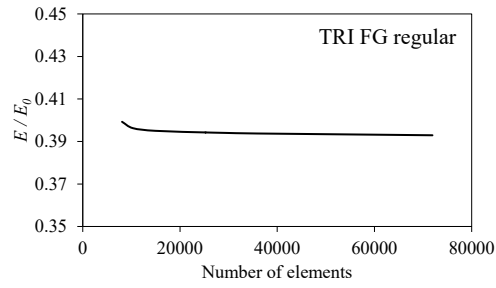


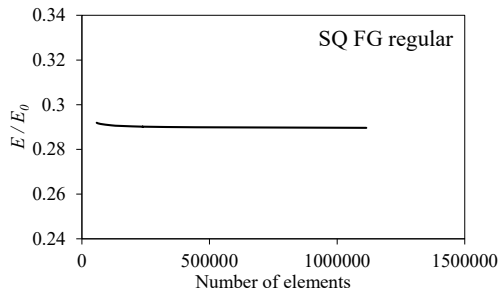
Figure B.11. The calibrated correction factor, η as a function of the degree of irregularity, Δ , for HEX, TRI, and SQ honeycombs, obtained from FE simulations based on the 2D Timoshenko beam model.



((a))



((b))



((c))

Figure B.12. The mesh sensitivity analysis for the 2D plane-stress models. a) HEX, b) TRI, and c) SQ lattice structures.

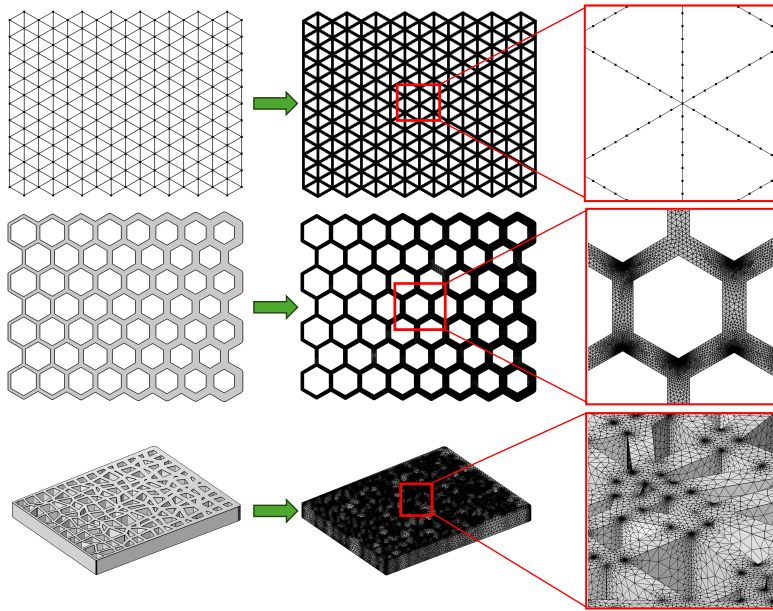


Figure B.13. Examples of the three FE models we utilized. The 2D Timoshenko beam model for uniform TRI geometry, the 2D plane-stress solid FE model for FG regular HEX geometry, and the 3D solid FE model for the FG irregular SQ geometry.

B.2 Supplementary Table

Table B.1. The coefficient A_0 to A_5 in Table 2.2 for the correction factor κ .

	m	A_0	A_1	A_2	A_3	A_4	A_5
HEX	1	0.583	1.0056	-0.7963	0.2444	-0.0354	0.002
	2	0.4148	1.3933	-1.0996	0.3428	-0.0502	0.0029
	3	0.4148	1.3933	-1.0996	0.3428	-0.0502	0.0029
TRI	1	1.081	-0.1236	0.0587	-0.0204	0.0034	-0.0002
	2	1.1254	-0.2246	0.1379	-0.0481	0.0078	-0.0005
	3	1.1604	-0.3076	0.2036	-0.0695	0.011	-0.0007
SQ	1	1.0197	-0.0004	-0.0254	0.0066	-0.0007	0.00003
	2	1.0377	-0.0412	0.0076	-0.0062	0.0014	-0.0001
	3	1.0583	-0.091	0.0479	-0.0195	0.0034	-0.0002

APPENDIX C

Adjusting Impact-Induced Wave Propagation in Elastic 2D Lattice Structures through Cell Geometry, Random Irregularity, and Mass Redistribution

C.1 Geometric models for 118 different 2D lattice designs

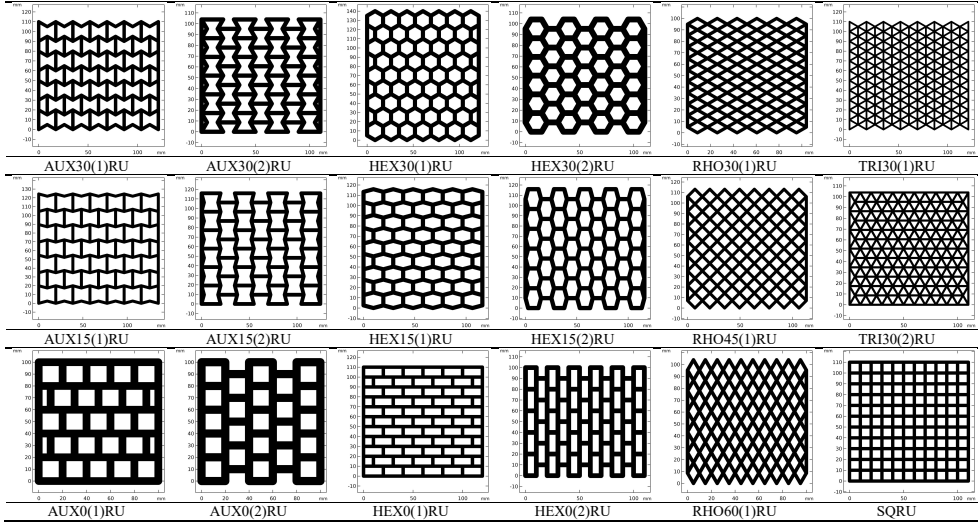


Figure C.1. The regular uniform (RU) lattice structures for analyzing the wave propagation from right to left.

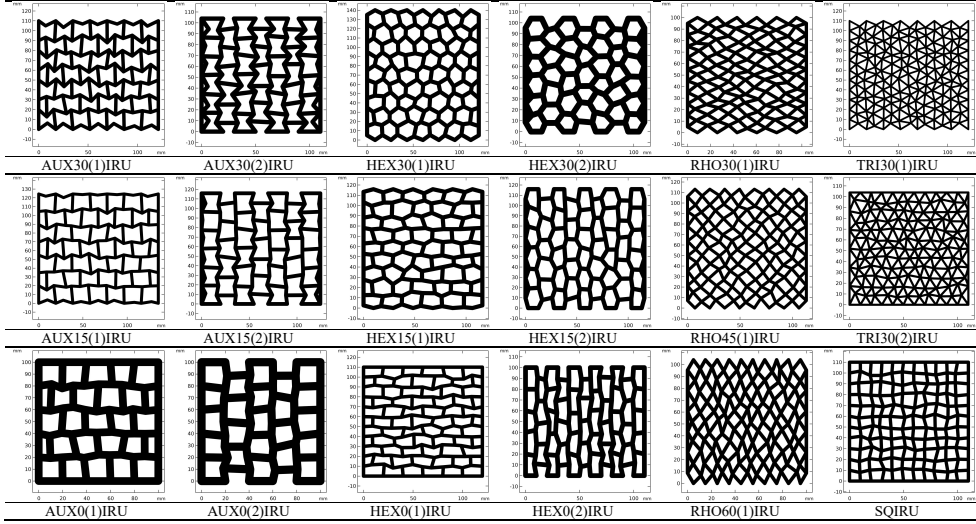


Figure C.2. The irregular uniform (IRU) lattice structures for analyzing the wave propagation from right to left.

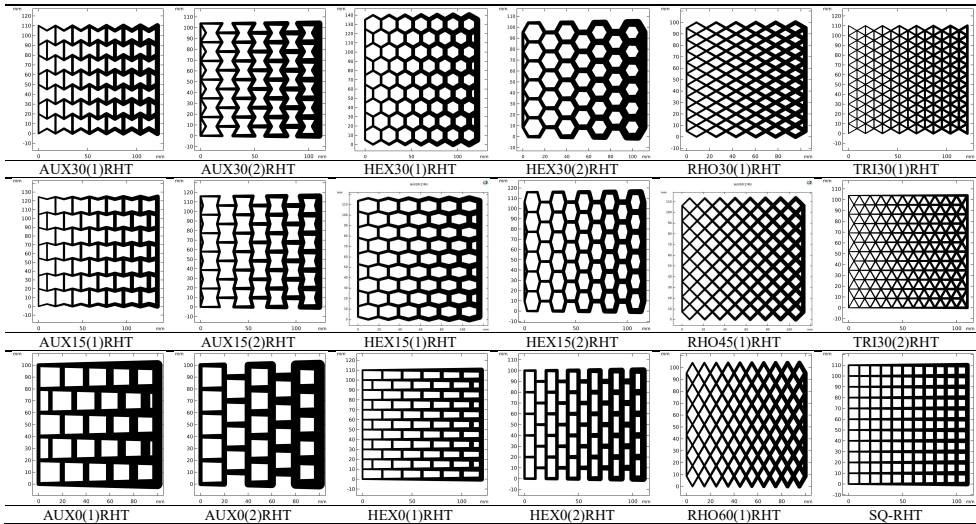


Figure C.3. The regular heavy-tip (RHT) lattice structures for analyzing the wave propagation from right to left. The corresponding regular light-tip (RLH) configurations are obtained by a 180° rotation of the heavy-tip (RHT) structures.

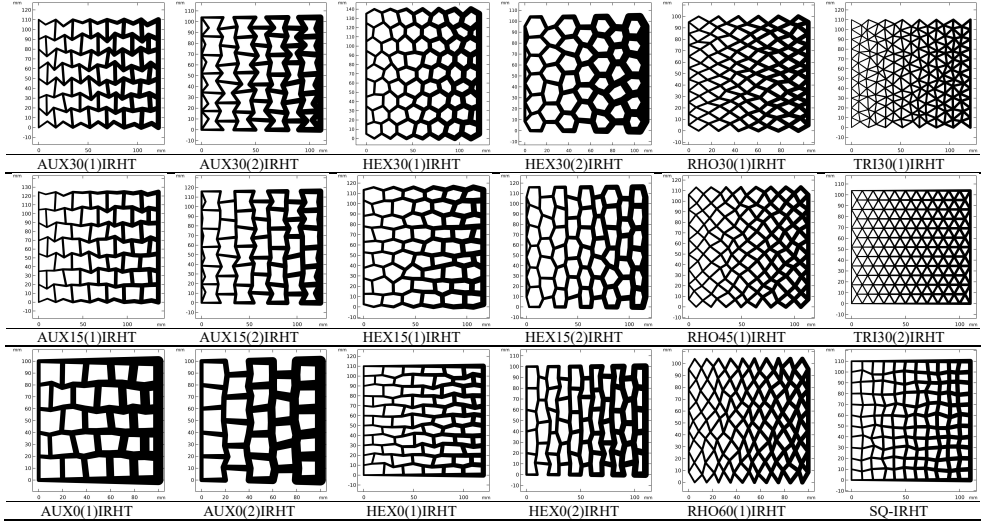


Figure C.4. The irregular heavy-tip (IRHT) lattice structures for analyzing the wave propagation from right to left.

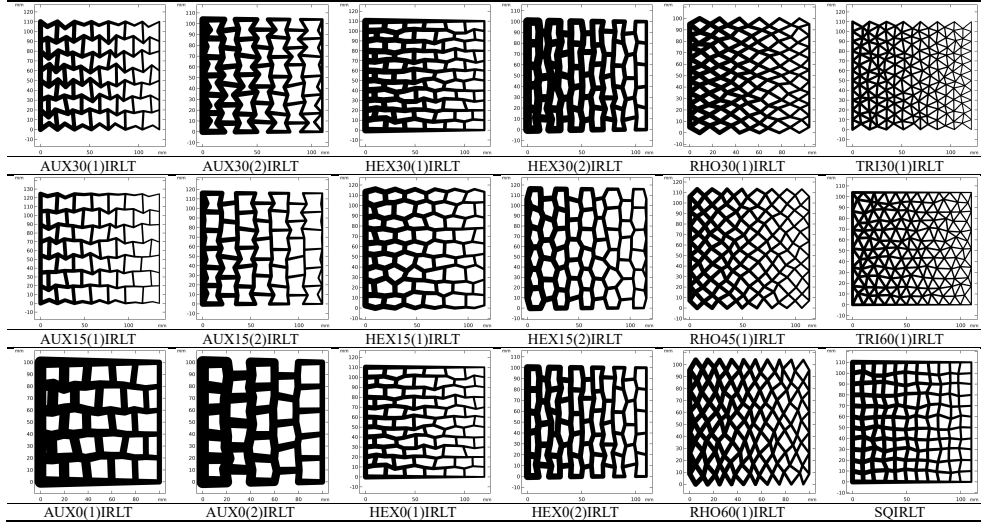


Figure C.5. The irregular light-tip (IRLT) lattice structures for analyzing the wave propagation from right to left.

APPENDIX D

Physically based machine learning for the multi-objective optimal design of partially recycled materials: The case study of rubber resources in the automotive industry

D.1 Closed-Form Solution for the Case of Two Recovery Properties and Two ADs

Here the closed-form expressions for the simplest case of multi-AD recovery, where the number of recovery properties and the number of ADs are both equal to 2 are presented. In this case, the matrix $[A]$ in Eq. 14 becomes the smallest possible square matrix, giving a simple expression for $[A]^{-1}$. Consequently, the expression for the volume fractions $\bar{v}_1$ and $\bar{v}_2$ in terms of deviations δ_1 and δ_2 can be derived as follows:

$$\bar{v}_1 = \frac{Q_1\delta_1 + Q_2\delta_2 + Q_3\delta_1\delta_2 + Q_4}{\chi}, \quad (\text{D.1a})$$

$$\bar{v}_2 = \frac{Q_5\delta_1 + Q_6\delta_2 + Q_7\delta_1\delta_2 + Q_8}{\chi}, \quad (\text{D.1b})$$

$$\chi = Q_9\delta_1 + Q_{10}\delta_2 + Q_{11}\delta_1\delta_2 + Q_{12}. \quad (\text{D.1c})$$

where,

$$Q_1 = \eta_{12} \frac{q_2}{\lambda_1} - \eta_{22} \frac{q_4}{\lambda_1}, \quad (\text{D.2a})$$

$$Q_2 = \eta_{12} \frac{q_6}{\lambda_2} - \eta_{22} \frac{q_1}{\lambda_2}, \quad (\text{D.2b})$$

$$Q_3 = \frac{(\eta_{22} - \eta_{12})}{\lambda_1 \lambda_2}, \quad (\text{D.2c})$$

$$Q_4 = \eta_{22} q_1 q_4 - \eta_{12} q_2 q_6, \quad (\text{D.2d})$$

$$Q_5 = \eta_{21} \frac{q_5}{\lambda_1} - \eta_{11} \frac{q_2}{\lambda_1}, \quad (\text{D.3a})$$

$$Q_6 = \eta_{21} \frac{q_1}{\lambda_2} - \eta_{11} \frac{q_3}{\lambda_2}, \quad (\text{D.3b})$$

$$Q_7 = \frac{(\eta_{11} - \eta_{21})}{\lambda_1 \lambda_2}, \quad (\text{D.3c})$$

$$Q_8 = \eta_{11} q_2 q_3 - \eta_{21} q_1 q_5, \quad (\text{D.3d})$$

$$Q_9 = \frac{\eta_{12} \eta_{21} q_5 - \eta_{11} \eta_{22} q_4}{\lambda_1}, \quad (\text{D.4a})$$

$$Q_{10} = \frac{\eta_{12} \eta_{21} q_6 - \eta_{11} \eta_{22} q_3}{\lambda_2}, \quad (\text{D.4b})$$

$$Q_{11} = \frac{(\eta_{11} \eta_{22} - \eta_{12} \eta_{21})}{\lambda_1 \lambda_2}, \quad (\text{D.4c})$$

$$Q_{12} = \eta_{11} \eta_{22} q_3 q_4 - \eta_{12} \eta_{21} q_5 q_5, \quad (\text{D.4d})$$

in which,

$$q_1 = \frac{1}{\lambda_1} - 1, \quad (\text{D.5a})$$

$$q_2 = \frac{1}{\lambda_2} - 1, \quad (\text{D.5b})$$

$$q_3 = \xi_{11} + \frac{1}{\lambda_1}, \quad (\text{D.5c})$$

$$q_4 = \xi_{22} + \frac{1}{\lambda_2}, \quad (\text{D.5d})$$

$$q_5 = \xi_{21} + \frac{1}{\lambda_2}, \quad (\text{D.5e})$$

$$q_6 = \xi_{12} + \frac{1}{\lambda_1}. \quad (\text{D.5f})$$

$$(\text{D.5g})$$

Then, one can substitute these volume fractions into Eq. 9 to obtain the corresponding cost ratio of recovery as a function of deviations, δ_1 and δ_2 , as well:

$$F_{\S} = \lambda_{\S} (Q_{\S1} \delta_1 + Q_{\S2} \delta_2 + Q_{\S3} \delta_1 \delta_2 + Q_{\S4}), \quad (\text{D.6})$$

where,

$$\begin{Bmatrix} Q_{\S1} \\ Q_{\S2} \\ Q_{\S3} \\ Q_{\S4} \end{Bmatrix} = \begin{bmatrix} Q_1 & Q_5 \\ Q_2 & Q_6 \\ Q_3 & Q_7 \\ Q_4 & Q_8 \end{bmatrix} \begin{Bmatrix} q_{\S1} \\ q_{\S2} \end{Bmatrix}. \quad (\text{D.7})$$

and,

$$q_{\$1} = r_{\$1} - 1 \quad (\text{D.8a})$$

$$q_{\$2} = r_{\$2} - 1 \quad (\text{D.8b})$$

Note that the coefficients Q_i and $Q_{\$i}$ are functions of $\{r_{ij}\}$, $\{\xi_{ij}\}$, $\{\lambda_i\}$, and $\{r_{\$j}\}$.

D.2 Parametric study on the required volume fractions of ADs for a full recovery

Here a parametric problem of full recovery of two properties, utilizing two ADs ($N_p = N_a = 2$) is examined. To evaluate the required volume fractions of AD1 and AD2, $\bar{v}_1$, and $\bar{v}_2$, it is assumed that:

- *The property ratios:* Properties 1 and 2 of AD1 and AD2 are 10 times those of the recycled matrix, respectively, i.e., $r_{11} = r_{22} = 10$. The mutual ratios r_{12} and r_{21} , representing the effect of AD2 on property 1 and AD1 on property 2, are equal and vary within $0.5 \leq r_{12} = r_{21} \leq 1$. At $r_{12} = r_{21} = 1$, AD1 has no impact on property 2 and AD2 has no effect on property 1. At $r_{12} = r_{21} = 0.5$, property 1 of AD2 and property 2 of AD1 are 50% weaker than the recycled matrix.
- *The recycling efficiency:* λ_2 varies across values of 0.5, 0.6, 0.7, 0.8, and 0.9. For each specific λ_2 , the recycling efficiency λ_1 of property 1 is progressively reduced from its maximum value of 1 until the condition $\bar{v}_1 + \bar{v}_2 \leq 1$ is met.
- *The packing fitting parameter:* Since the H-T model spans between the ROM and IROM extremes, properties 1 and 2 are assumed to adopt either ROM or IROM conditions, resulting in three extreme combinations: both ROM (all four ξ_{ij} set to infinity), both IROM (all four ξ_{ij} set to zero), and ROM-IROM where property 1 follows ROM ($\xi_{11} = \xi_{12} = \infty$) while property 2 obeys IROM ($\xi_{21} = \xi_{22} = 0$).
- *The deviation:* Full recovery is assumed, resulting in both deviations being set to zero: $\delta_1 = \delta_2 = 0$.
- *The solution:* Since there are two ADs, we use Eqs. S1 to S5 to obtain $\bar{v}_1$, and $\bar{v}_2$.

Figure D.1 plots $\bar{v}_1$ versus $\bar{v}_2$ for three combinations of ROM and IROM models. Consider the dashed horizontal lines in the graphs, indicating when $r_{12} = r_{21} = 1$. Across all combinations, as λ_1 decreases from 1 (moving left to right in the graphs), $\bar{v}_1$ gradually increases to compensate for the drop in property 1. With $r_{21} = 1$, the addition of AD1 doesn't affect property 2, keeping $\bar{v}_2$ constant. Notably, for a given λ_1 , ROM requires a lower $\bar{v}_1$ for complete recovery compared to IROM. As r_{12} (and r_{21} , assumed equal here) gradually decreases, increasing each volume fraction aids in one property's recovery but leads to a corresponding decline in the other property. For a given λ_2 , to offset the loss in property 1, $\bar{v}_1$ needs to increase, causing a further decline in property 2. This mutual weakening effect can be counteracted by re-adjusting $\bar{v}_2$, resulting in optimal $\bar{v}_1$ and $\bar{v}_2$ values for complete recovery of both properties.

Since in this parametric study, property enhancement with a factor of 10 and reciprocal property reduction with a maximum factor of 0.5 are considered, the addition

of ADs improves the properties of the recycled matrix, in an overall sense. However, if the enhancing effects of ADs are minimal and/or the mutual weakening effect is significant, an optimal solution may not exist (resulting in negative optimal volume fractions or a sum exceeding one), indicating that the selected ADs are unsuitable. In Figure D.1(b), where the micromechanics model is IROM, yielding a significantly lower recovery effect compared to ROM, the mutual weakening ratios are limited to 0.8 instead of 0.5 to ensure the feasibility of the optimal volume fractions. As a system of linear equations, a solution is not feasible as well when $\det(A) = 0$ in Eq. 14, unless all equations become independent, indicating identical recovery functions for all the properties. This implies an infinite number of optimized combinations. To illustrate, consider the special case where matrix $[A]$ is 2×2 and both properties follow the ROM. In this scenario, if $(r_{11} - 1)/(r_{22} - 1) = (r_{12} - 1)/(r_{21} - 1) = (1/\lambda_1 - 1)/(1/\lambda_2 - 1)$, infinite pairs of optimal $\bar{v}_1$ and $\bar{v}_2$ exist, resulting in full recovery of both properties. When, $(r_{11} - 1)/(r_{22} - 1) = (r_{12} - 1)/(r_{21} - 1) \neq (1/\lambda_1 - 1)/(1/\lambda_2 - 1)$, there is no answer for Eq. 14.

D.3 Case Study of diversifying choices by increasing the number of ADs

This case study illustrates how incorporating additional ADs broadens recovery options, enhancing decision-making. It is assumed that:

- *The property ratios of ADs:* Five ADs, namely AD1 to AD5, can potentially contribute whose $\{r_{ij}\}$ vectors are listed in Table D.1 for recovery of two properties (property 1 and 2) of the recycled matrix.
- *The recycling efficiency:* are both fixed to 50% recovery efficiency, i.e., $\lambda_1 = \lambda_2 = 0.5$.
- *The packing fitting parameter:* effect of all ADs on both properties obeys ROM meaning that all ξ_{ij} is set to infinity.
- *The deviation:* Deviations for both the properties are assumed to be equal ranging from no recovery to full recovery, $0 \leq (\delta_1 = \delta_2) \leq 0.5$.
- *Relative cost of RM to VM:* is assumed to be 70%, resulting in $\lambda_s = 0.7$.
- *Relative cost of ADs to RM:* is assumed to be twice for all the ADS, i.e., $r_{sj} = 2$.

Since we are recovering two properties ($N_p = 2$), selecting two ADs among five from Table D.1 is sufficient which results in 10 possible pairs. Among them, the pairs AD1 + AD3 and AD2 + AD4, which do not contribute to the recovery of property 1 or property 2 respectively, do not lead to any solution. Additionally, since both properties are strengthened via the same micromechanical model, ROM, when AD5, which equally enhances both properties, is involved, the volume fraction of the other AD in the pair gets zero. Thus, all pairs including AD5 present the same result, and only the pair AD1 + AD5 is considered. Furthermore, AD2 + AD3 is excluded because it yields a solution identical to AD1 + AD4. These considerations reduce the number of AD pairs with feasible solutions from ten to four. To determine $\bar{v}_1$, $\bar{v}_2$, and the corresponding cost ratio of recycling, F_s , for these four selected pairs, one can utilize Eqs. S1 to S8.

Figure D.2(a) plots the calculated recovery cost ratio, F_s , as a function of deviations for the selected pairs of ADs. For all pairs, when the deviations are at their maximum value ($\delta_i = 0.5$), no ADs are introduced, and no recovery is performed. Consequently, the mixture solely consists of the RM, and $F_s = \lambda_s = 0.7$. As ADs are gradually added to the RM, deviations decrease, and the recovery cost ratio, F_s , increases. Complete recovery is achieved when both deviations reach zero. The required volume fraction of ADs for full recovery is shown in Figure D.2(b). Although full recovery is cost-saving for all AD pairs ($F_s < 1$), the pair AD3 + AD4, which requires the least volume fraction of ADs, is the most cost-effective choice.

After emerging AD3 + AD4 pair as the most cost-effective option, this absolute optimal pair is selected as the base, and a specified volume fraction v_3^+ from either AD5 or AD1 is gradually added to the base as the third supplemental AD⁺. Then, the recovery problem can be expressed as follows:

$$\begin{Bmatrix} \bar{v}_1 \\ \bar{v}_2 \\ \bar{v}_3 \end{Bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ 0 & 0 & 1 \end{bmatrix}^{-1} \begin{Bmatrix} b_1 \\ b_2 \\ v_3^+ \end{Bmatrix} \quad (\text{D.9})$$

Solving Equation (D.9), one can obtain the updated volume fractions $\bar{v}_1$, and $\bar{v}_2$ of AD3 and AD4 which are plotted in Figure D.2 (c) and (d) versus the volume fraction v_3^+ of supplemental AD5 and AD1, respectively. It is observed that adding AD5 to the AD3+AD4 pair leads to an equal decrease in both, and eventually, adding 25% of AD5 results in complete substitution. This leads to a 10.8% cost increase, as evident from the total volume fraction of ADs in Figure D.2(b). On the other hand, adding AD1 primarily replaces AD3 due to their similar role in recovering property 1. However, it reduces the volume fraction of AD4, albeit partially, because, unlike AD3, AD1 does not negatively affect property 2. Nevertheless, since AD1 has a lower recovery factor than AD3 (10 vs. 20 in Table D.1), the complete substitution results in a 5.3% increase in cost. This example demonstrates how substituting the optimal cost-effective combination with other alternatives can serve as a backup strategy, enabling full recovery with a minor increase in cost.

In the next example, all five ADs in Table D.1 are assumed to participate in the recovery process of two properties. It results in two recovery equations against five unknown volume fractions. In addition, here, we define a constraint on the price ensuring that the cost of the recovered material is precisely 80% of the VM ($F_{\$}=0.8$). Given the equal pricing of ADs, this condition equates to restricting the sum of volume fractions of ADs, leading to the third equation for the problem. Since the three available equations are fewer than the five variables, to find a solution, the AD1 and AD2 in Table D.1 are assumed as supplements and their volume fractions, v_1^+ and v_2^+ , are directly inserted into the problem within the range of 0 to 1 with a step of 0.025 leading to the following matrix form:

$$\begin{Bmatrix} \bar{v}_1 \\ \bar{v}_2 \\ \bar{v}_3 \\ \bar{v}_4 \\ \bar{v}_5 \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ A_{11} & A_{12} & A_{13} & A_{14} & A_{15} \\ A_{21} & A_{22} & A_{23} & A_{24} & A_{25} \\ A_{\$1} & A_{\$2} & A_{\$3} & A_{\$4} & A_{\$5} \end{bmatrix}^{-1} \begin{Bmatrix} v_1^+ \\ v_2^+ \\ b_1 \\ b_2 \\ b_{\$} \end{Bmatrix} \quad (\text{D.10})$$

where A_{ij} , b_i , and $b_{\$}$ are calculated from Table 1 (main text) for ROM model. By solving Equation (D.10), the volume fraction of the three remaining ADs, i.e., AD3, AD4, and AD5 are determined to achieve full recovery of two properties while satisfying the specified cost constraint. Despite the fact that for $N_a > N_p$ there could be an infinite number of solutions, since a step of 0.025 for entering the volume fractions of

AD1 and AD2 is chosen, six available distinct combinations are obtained which are depicted in Figure D.2(e) as representatives of multiple choices for the same recovery problem considering more ADs than properties. The smaller the steps of AD1 and AD2 changes are chosen, the number of possible choices increases.

D.4 Case Study of designing a single engineered AD for simultaneous recovery of all properties

This case study focuses on designing an exclusive single AD for the recovery of N_p properties. Consider the full recovery (no deviations) of four properties of an RM, with $N_p = 4$, each having a 50% recycling efficiency, $\lambda_i = 0.5$. The objective is to design an engineered AD that fully recovers all properties for a given critical volume fraction, v_{cri}^* . By substituting λ_i and the packing fitting parameters, ξ_{i1} , listed in Table D.3 for each property, into Eq. 16 (main text), the corresponding required property ratio of the AD for that property, r_{i1}^* , can be calculated for three different critical volume fractions of AD, $v_{cri}^* = 0.1, 0.3$, and 0.5 , as presented in Table D.3.

As expected, generally, a higher critical volume fraction of $v_{cri}^*=0.5$ necessitates smaller recovery ratios, r_{i1}^* , compared to a relatively low critical volume fraction of 0.1 while $v_{cri}^*=0.3$ stays between. When opting for a generous volume fraction of 0.5 , the engineered AD formulation should be designed to ensure that properties 1 to 4 of the AD are respectively 3, 4, 3.02, and 9 times those of the RM. It is revealed that property 1, governed by the robust ROM recovery model demands the least reinforcement. Conversely, property 4, following the weakest recovery model (IROM), necessitates the highest level of reinforcement, reaching up to 9 times that of RM. For properties 2 and 3, both recovered by the HT model, increasing the fitting parameter from $\xi = 2$ to $\xi = 100$ reduces the need for reinforcement. This occurs because higher ξ values approach the H-T model to the ROM. Besides, it is highlighted that when v_{cri}^* is as low as 0.1 , properties 2 and 4, following weaker recovery models of HT with $\xi = 2$ and IROM, cannot achieve full recovery whereas properties 1, and 3 can provide a full recovery with the engineered AD presenting reinforcing ratios as high as $r_{11}^*=11$, and $r_{31}^*=11.98$ even with $v_{cri}^*=0.1$.

D.5 Verification of the Optimization Algorithm

To validate the algorithm a sample recovery problem of an RM with two properties of interest, $N_p=2$, is defined as follows:

- *The recycling efficiencies:* They are 50% for both properties, meaning RM properties are half of the VM properties, $\lambda_1 = \lambda_2 = 0.5$.
- *The cost of the RM:* It is assumed to be half of VM, leading to a recycling cost ratio of $\lambda_{\S}=0.5$.
- *The property ratio of ADs:* Five ADs namely AD1 to AD5, can potentially contribute to the recovery process whose property ratios to RM, $\{r_{ij}\}$, are listed in Table D.1. AD1 and AD2 are engineered to exclusively recover one property without affecting the other. AD3 and AD4 provide high recovery in one property by weakening another. Lastly, AD5 uniformly and moderately recovers both properties.
- *The cost of ADs:* All ADs are assumed to be twice as expensive as the RM, i.e., $r_{\S j} = 2$.
- *The packing fitting parameters:* Three distinct values, 2, 20, and 200, are considered for the fitting parameter of each property, ξ_{1j} and ξ_{2j} . These values represent a progressive increase in the influence of ADs on the recovery of properties. Consequently, a total of 9 possible combinations are obtained for the recovery of the two properties. In every combination of ξ_{1j} and ξ_{2j} , it is assumed that the packing fitting parameters of all ADs are identical for each property.
- *Objective Functions:* Three objective functions are considered, including the two individual deviations from VM, δ_1 and δ_2 , as well as the recovery cost ratio, $F_{\S}$.
- *Constraints:* No constraints are imposed for the feasibility of comparison to the analytical solution obtained from Eqs. S1 to S8.

Since we are interested in two properties, any pair of ADs from Table D.1 may be sufficient to recover them. Choosing two among five yields 10 possible pairs. However, AD1 + AD3 and AD2 + AD4 do not contribute to the recovery of property 1 and property 2, respectively, and are therefore excluded from the analysis. This reduces the number of pairs to 8. As the reference for validation, we first extract the analytical solution for each pair of ξ_{1j} and ξ_{2j} following these four steps:

1. For every available pair of ADs, the recycling cost ratio is evaluated using Equation (D.6) as a function of deviations, $F_{\S}(\delta_1, \delta_2)$.
2. The recycling cost ratio, $F_{\S}(\delta_1, \delta_2)$, is visualized as a 3D surface plot in Cartesian coordinates, where deviations δ_i vary from 0, indicating 100% recovery, to $(1 - \lambda_i) = 0.5$, indicating no recovery.

3. In every (δ_1, δ_2) point, among eight surfaces corresponding to eight AD pairs, the one with the minimum cost ratio, $F_{\S}$, is chosen, to identify the surface with minimum recovery cost across the entire range of deviations.
4. The volume fraction of ADs corresponding to the emerged surface with minimal recovery cost are calculated using Equation (D.1).

On the other hand, for the numerical optimization algorithm, there is no limit on the number of ADs; for each pair of ξ_{1j} and ξ_{2j} , the algorithms free to use any combinations of five ADs from Table D.1 to minimize three objective functions, including δ_1 , δ_2 , and $F_{\S}$. No constraints are applied to the objective functions, except that the sum of the volume fractions of ADs does not exceed one, $v_T \leq 1$. Figure D.3(a)-(i) displays the optimized objective functions from the numerical optimization algorithm, represented as 3D Pareto fronts (green dots), for nine different combinations of the H-T fitting parameters, ξ_{1j} and ξ_{2j} . For comparison, the corresponding 3D surface plots derived from the reference analytical solutions are also presented in the same 3D Cartesian coordinates. A high level of agreement is observed between the numerical Pareto fronts and the minimum analytical surfaces, confirming the accuracy and efficiency of the MO optimization algorithm for the recovery of recycled resources through the addition of ADs. Note that in Figure D.3 the percentage of recovery for property i -th is defined as, $(1 - \frac{\delta_i}{1-\lambda_i}) \times 100$.

For further investigation, Figure D.4(a)-(i) compares the volume fractions of AD pairs used by the analytical approach, corresponding to the minimal surfaces (solid bars), with the volume fractions of ADs obtained by the numerical optimization algorithm (hatched bars), corresponding to the Pareto front of minimum objective functions. Interestingly, despite the numerical algorithm having the freedom to use all five ADs to minimize the objective functions, it consistently selects the same pair of ADs corresponding to the minimal surfaces obtained from the analytical solution. Moreover, the volume fraction of each AD in the selected pair closely matches the analytical solution with acceptable accuracy. This demonstrates the numerical algorithm's capability and precision in identifying suitable ADs for optimal and cost-effective recovery from a diverse library of available ADs.

After validation of the optimization algorithm, let us analyze the results further. As shown in Figure D.3, with an increase in the recovery percentage of either of the properties (decreasing the deviation from VM), the recovery cost increases. Therefore, in all Pareto fronts, the highest recovery cost occurs at point A, where both properties are fully recovered. Conversely, the lowest recovery cost is at point I, where no recovery has taken place (no AD has been added) and the mixture consists only of RM, resulting in $F_{\S} = \lambda_{\S} = 0.5$. Moreover, the results indicate that, in general, the cost of recovery decreases with an increase in the H-T fitting parameters, ξ_{1j} and ξ_{2j} . This is because higher ξ_{ij} values enhance the effectiveness of the ADs in the recovery of RM, resulting in a lower required volume fraction of ADs and consequently reducing the overall cost of recovery. It is also evident that when the fitting parameters are not equal for two properties, $\xi_{1j} \neq \xi_{2j}$, the property with the larger value requires less

cost for full recovery than the other property, resulting in an asymmetrical recovery process. For example, in Figure D.3(g) where $\xi_{1j} = 200$ and $\xi_{2j} = 2$, point C, which corresponds to the full recovery of the property 1 without recovering the property 2, requires a lower volume fraction of AD and, consequently, a lower recovery cost compared to point G and vice versa.

Since all ADs are priced equally, the recovery cost is proportional to the total volume fraction of ADs, represented by the height of the bar graphs in Figure D.4. Consequently, as the H-T fitting parameters increase, the height of these bars gradually decreases. Moreover, it is observed that among the five available ADs, only AD3, AD4, and AD5 are utilized for optimal recovery, while AD1 and AD2 are always excluded. Analysis from Table D.1 reveals that AD3 and AD4 exhibit significant capability in enhancing properties 1 and 2, respectively, despite their mutual weakening impact on the recovery of the other property. In contrast, AD1 and AD2 do not present any weakening recovery but offer lower recovery potential compared to AD3 and AD4 (10 vs 20). The optimization algorithm therefore favors AD3 and AD4, utilizing AD5 to offset their mutual weakening effect since AD5 contributes moderately to the recovery of both properties equally. Consequently, AD5 participates in optimal recovery when the fitting parameter of H-T is small. As ξ_{1j} and ξ_{2j} increase, enhancing the impact of ADs in recovery, the need for AD5 diminishes (blue bars in Figure D.4), and AD3 (Green bars) and AD4 (yellow bars) independently achieve the desired recovery across the entire range of target deviations.

D.6 Supplementary Figures

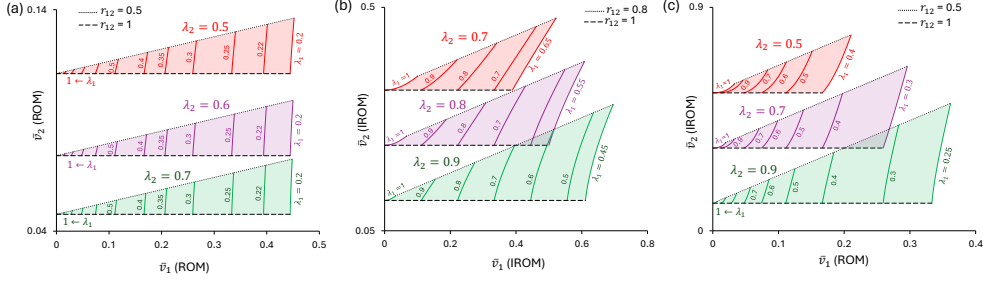


Figure D.1. A parametric study for recovery problem of two ADs and two properties of interest. The volume fraction of ADs, $\bar{v}_1$, and $\bar{v}_2$, for a wide range of recycling efficiencies, λ_1 and λ_2 and different combinations of ROM and IROM micromechanics models. It is assumed that $r_{11}=r_{22}=10$ and $0.5 \leq r_{12} = r_{21} \leq 1$ while targeting a full recovery with no deviations, $\delta_1 = \delta_2 = 0$.

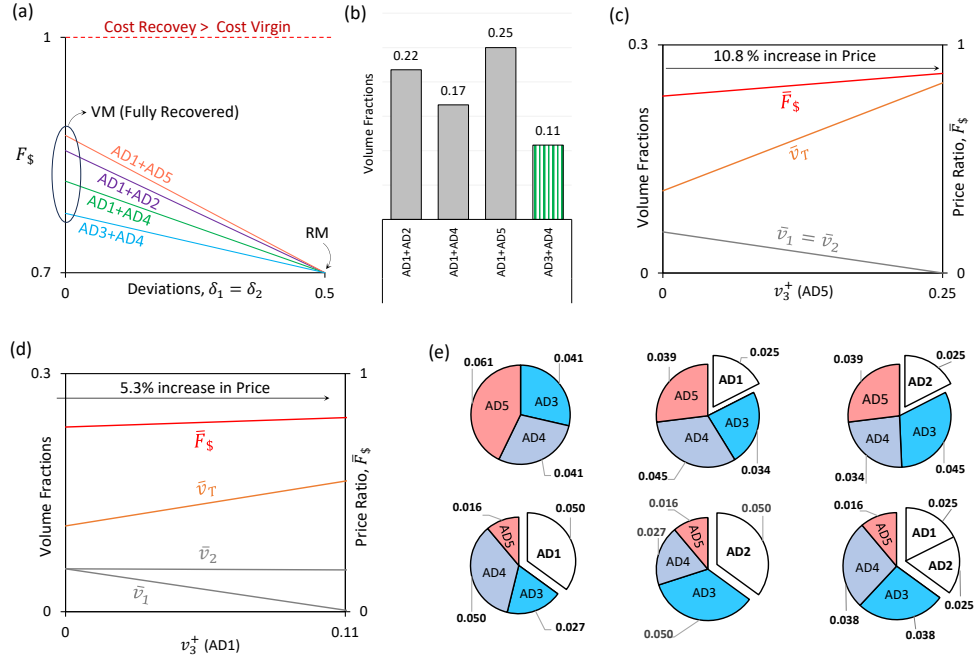


Figure D.2. Expanding the circle of choices by including supplementary ADs. (a) The recovery cost ratio, F_s , versus the deviations, $0 \leq (\delta_1 = \delta_2) \leq 0.5$, for the four selected pairs of ADs, identifying AD3 + AD4 as the most economical option. (b) The corresponding total volume fractions of AD pairs for full recovery of properties. As all the ADs are assumed to have a price twice that of RM, a higher total volume fraction results in a higher recovery cost. (c) Gradually addition of AD5 to the optimal AD2+AD3 pair from volume fraction 0 to 0.25 obtained by Equation (D.9) resulting in a full replacement of ADs with 10.8% increase in cost, (d) Gradually addition of AD1 to the optimal AD2+AD3 pair from volume fraction 0 to 0.114 resulting in the replacement of AD3 by AD2 at a cost increase of 5.3%, (e) six possible ADs combinations of the same price ratio of $\bar{F}_s = 0.8$ obtained from Equation (D.10). Note: $\lambda_s = 0.7$, and $\lambda_1 = \lambda_2 = 0.5$.

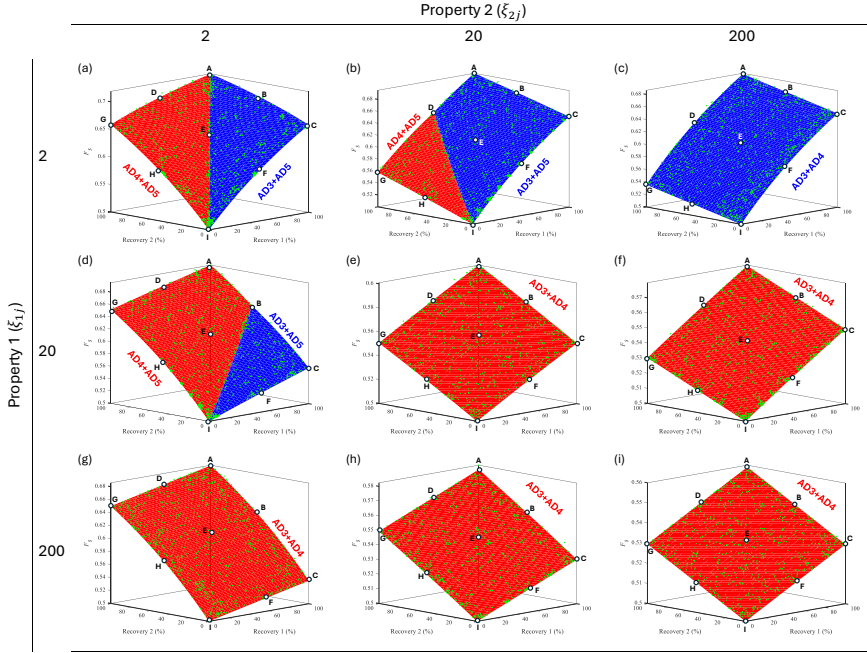


Figure D.3. Validation study of the numerical optimization algorithm, Pareto Fronts of the objective functions. Comparison between the Pareto fronts of three objective functions—deviations δ_1 and δ_2 , and the recovery cost ratio F_s —shown as green dots, with the analytical minimal surfaces obtained from Eqs. S1 to S8, depicted as solid blue and red surfaces. The study examines nine different combinations for the two recovered properties, assigning three values (2, 20, and 200) to the H-T fitting parameters ξ_{1j} and ξ_{2j} . Note: the recovery percentage of property i -th is defined as, $(1 - \frac{\delta_i}{1-\lambda_i}) \times 100$.

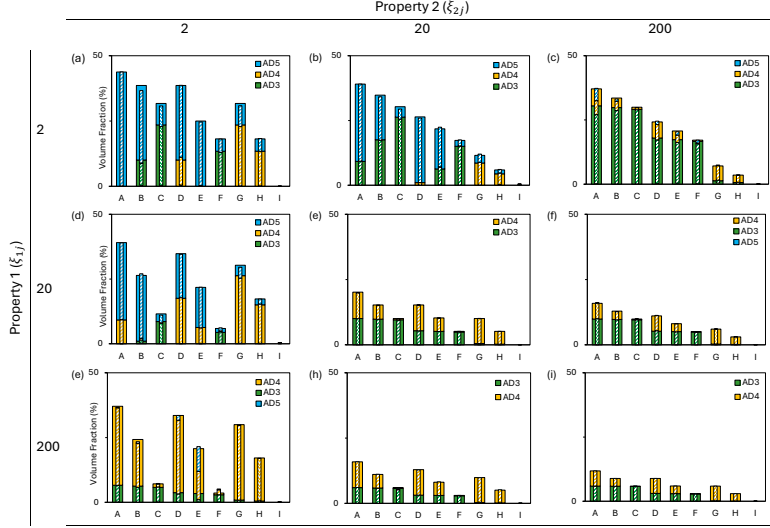


Figure D.4. Validation study of the numerical optimization algorithm, the volume Fractions of ADs. The comparison between the volume fractions of AD pairs calculated from the analytical approach, corresponding to the minimal surfaces (solid bars), with the volume fractions of ADs obtained by the numerical optimization algorithm (hatched bars), corresponding to the Pareto front of minimum objective functions for nine different combinations of ξ_{1j} and ξ_{2j} , presented in Figure D.3.

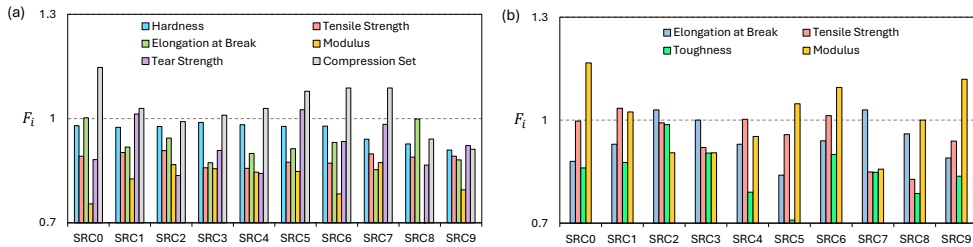


Figure D.5. The evaluated recovery factors from experiments. The recovery functions, F_i , (the property ratio of SRC-VM blend to VM) calculated from experimental tests. (a) SRCs blended to VM1, (b) to VM2.

D.7 Supplementary Tables

Table D.1. The property ratios, r_{ij} , of sample ADs (AD1 to AD5) for two sample properties of interest. It is defined to be used as the input of the case study in Appendix D.3 and the verification study in Appendix D.5.

j	ADs	$\frac{r_{ij}}{i}$	
		1	2
1	AD1	10	1
2	AD2	1	10
3	AD3	20	0.5
4	AD4	0.5	20
5	AD5	5	5

Table D.2. A sample of an engineered single AD for multiple full recovery of properties.. The property ratio, r_{i1}^* , of the exclusively designed AD in Appendix D.4, for the simultaneous full recovery (no deviations) of four properties, each with a 50% recycling efficiency ($\lambda_i = 0.5$). The property ratios, r_{i1}^* , are listed for three different critical volume fractions of AD ($v_{cri}^* = 0.1, 0.3, \text{ and } 0.5$), given the packing fitting parameter ξ_{i1} for each property.

Property		v_{cri}^*		
		0.1	0.3	0.5
i	ξ_{i1}	r_{i1}^*		
1	∞ (ROM)	11	4.33	3
2	2	-	16	4
3	100	11.98	4.41	3.02
4	0 (IROM)	-	-	9

Table D.3. The back-calculated property ratios, r_{ij} , for the SRCs blended with VM1, used in the case study of spring pads.

		r_{ij}					
		i					
		1	2	3	4	5	6
j	SRCs	Hardness	Tensile strength	Elongation	Modulus	Tear strength	Comp. Set
1	SRC0	0.90	0.53	1.01	0.08	0.49	1.91
2	SRC1	0.89	0.59	0.74	0.44	0.33	0.96
3	SRC2	0.89	0.45	0.69	0.16	0.70	1.50
4	SRC3	0.88	0.57	0.63	0.29	1.07	1.15
5	SRC4	0.60	0.53	0.49	0.19	0.65	0.61
6	SRC5	0.73	0.55	0.39	0.46	0.92	1.50
7	SRC6	0.91	0.40	0.56	0.36	0.35	1.15
8	SRC7	0.67	0.52	0.99	-0.09	0.43	0.73
9	SRC8	0.89	0.46	0.61	0.37	1.13	1.44
10	SRC9	0.94	0.40	0.46	0.39	0.59	1.05

Table D.4. The back-calculated property ratios, r_{ij} , for the SRCs blended with VM2, used in the case study of car tires.

		r_{ij}			
		i			
		1	2	3	4
j	SRCs	Tensile strength	Elongation	Modulus	Toughness
1	SRC0	0.97	0.12	4.33	0.11
2	SRC1	1.38	0.42	1.25	0.66
3	SRC2	0.92	1.33	0.26	1.24
4	SRC3	0.36	1.00	0.26	0.36
5	SRC4	1.03	0.42	0.58	0.44
6	SRC5	0.62	-0.08	1.56	-0.23
7	SRC6	1.14	0.49	2.33	0.58
8	SRC7	-0.04	1.33	0.00	0.09
9	SRC8	-0.14	0.64	1.00	-0.27
10	SRC9	0.48	0.17	2.85	-0.10

APPENDIX E

Implementation and Preliminary Assessment of MOC, GMC, and HFGMC

Abstract:

This chapter presents an exploratory study of micromechanical methods, namely the method of cells, the generalized method of cells, and the high-fidelity generalized method of cells. These approaches, originally developed for predicting the effective mechanical properties of composite materials, were examined with the perspective of integrating them into machine learning frameworks, particularly in combination with image processing techniques. The aim was to assess their potential for generating structured datasets that could later be exploited in predictive modeling or failure analysis of representative unit cells. Although the methods themselves were not further developed, existing codes were carefully studied, implemented, and optimized to improve computational performance. This exercise not only provided preliminary numerical results but also offered valuable training in computational modeling and programming. In particular, the analytical–computational hybrid nature of these methods made them an effective entry point for learning advanced coding in Python and Julia, skills that were subsequently crucial for the research presented in the following chapters. Therefore, this work should be seen as a methodological exploration that, while not directly leading to publications, significantly contributed to the technical foundation and computational expertise required for the later machine learning–oriented investigations of this dissertation.

Highlights:

- Explored micromechanical methods for potential integration with machine learning.
- Implemented and optimized existing codes to assess computational performance.
- Produced preliminary numerical results as proof of concept.
- Gained essential programming experience in Python and Julia through these methods.
- Established the technical groundwork for subsequent machine learning research.

keywords: Method of Cells, Generalized Method of Cells, High-Fidelity Generalized Method of Cells, Micromechanics, Synthetic Data, Machine Learning.

E.1 Introduction

Composite materials are widely used in engineering applications due to their high strength-to-weight ratio and tunable mechanical properties [4]. Accurate prediction of their effective mechanical behavior requires careful modeling of the microstructure, which is often represented by a Representative Volume Element (RVE) or a Representative Unit Cell (RUC) [164–166]. These elements exploit the periodicity of the microstructure to reduce the computational domain while capturing the essential mechanical responses of the material. Traditionally, the Finite Element Method (FEM) applied to RVEs has been the standard approach for determining effective properties and failure behavior, but FEM can become computationally expensive for parametric studies, large ensembles of microstructures, or cases requiring repeated simulations for data generation. Semi-analytical micromechanical methods, such as the Method of Cells (MOC), the Generalized Method of Cells (GMC), and the High-Fidelity Generalized Method of Cells (HFGMC), provide an efficient alternative by discretizing the RUC into subcells and coupling analytical formulations with numerical computation [167–169]. This approach leverages the periodicity of the RUC and allows each subcell to behave as an individual unit with local material properties, enabling faster calculations while still capturing key mechanical behavior [170–172]. Moreover, the structured discretization resembles a pixel-like grid, naturally suggesting potential applications in machine learning for predictive modeling and data-driven analysis. Motivated by these advantages, this chapter explores the implementation and preliminary assessment of MOC, GMC, and HFGMC, focusing on evaluating their feasibility for data generation and providing a computational foundation for subsequent machine learning studies, rather than developing new theoretical formulations.

The micromechanical methods considered in this study—MOC, GMC, and HFGMC—share a common foundation in representing a composite microstructure through the discretization of a RUC into an array of subcells. MOC, introduced as one of the earliest approaches, provides closed-form relations for average stress and strain fields in each subcell, making it efficient but limited in accuracy when dealing with complex stress states. The GMC extended this framework by introducing more rigorous displacement and traction continuity conditions between subcells, significantly improving accuracy while retaining computational efficiency. The HFGMC further enhanced the approach by incorporating higher-order displacement fields within each subcell, thereby enabling the capture of local stress and strain gradients with much greater precision, at the cost of additional computational effort. Together, these methods form a hierarchy of micromechanical models, balancing accuracy and efficiency. Given their ability to exploit periodicity, handle heterogeneous materials, and discretize microstructures in a structured, image-like manner, they are well-suited for both classical micromechanics and, potentially, for generating structured datasets in machine learning applications. Detailed formulations of these methods can be found in the foundational works of Aboudi and co-authors [173], and will not be repeated here; instead, this chapter focuses on their implementation, computational perfor-

mance, and exploratory use in the context of data generation.

Despite the extensive literature and established nature of MOC, GMC, and HFGMC, their implementation in the present work was motivated by several considerations. First, these methods provide a computationally efficient alternative to finite element simulations, making them attractive for generating structured datasets suitable for training and validating machine learning models. Their subcell-based discretization, which resembles a pixelated grid, aligns naturally with image-processing techniques, opening opportunities to integrate micromechanical modeling with data-driven approaches. Second, in order to apply these methods effectively to data-centric tasks, it was necessary to study, implement, and in some cases adapt existing codes, with the dual objectives of improving computational performance and making the outputs compatible with machine learning workflows. Finally, this stage of research served as a crucial training ground: the hybrid analytical–computational character of these methods offered a clear and systematic entry point for learning advanced programming in Python and Julia, which later became essential for the development of more sophisticated simulation and machine learning pipelines presented in subsequent chapters. Thus, the motivation for this chapter lies not in advancing the theoretical formulations of the methods themselves, but in assessing their feasibility for new applications and consolidating the computational skills required for the next stages of this dissertation.

The primary objectives of this chapter are therefore threefold. First, to implement and review existing computational codes for MOC, GMC, and HFGMC, with particular attention to their numerical performance and practical usability. Second, to produce and analyze preliminary results that illustrate the potential of these methods for efficient data generation in micromechanics. Third, to document the role of this exploratory study in developing the computational expertise and programming skills that form the foundation for the machine learning–oriented investigations presented in the following chapters. By pursuing these objectives, the chapter establishes both the methodological context and the technical preparation for the subsequent contributions of this dissertation.

It is important to clarify the scope and limitations of this chapter. The focus is on implementation, performance assessment, and preliminary exploration, rather than on developing new theoretical formulations of MOC, GMC, or HFGMC. While these methods have been extensively studied in the literature, this work primarily investigates their feasibility for generating structured datasets and for providing a practical learning platform in computational modeling. Consequently, detailed derivations, advanced theoretical extensions, or extensive validation studies are beyond the scope of this chapter. Nevertheless, the insights gained through code adaptation, computational optimization, and the systematic exploration of method capabilities provide a meaningful contribution, both as a methodological reference and as a foundation for the machine learning–oriented studies presented in subsequent chapters.

E.2 Implementations and Formulations

To investigate the potential of semi-analytical micromechanical methods as efficient data generators for machine learning applications, three representative approaches, namely the MOC, the GMC, and the High-Fidelity HFGMC, were implemented and studied. Although the theoretical basis of these approaches is well established in the literature [173], a brief overview is provided here to establish notation and ensure the chapter remains self-contained. Emphasis is placed not on re-deriving the full mathematical framework, but on clarifying the role of the RUC, its discretization into subcells, and the subsequent formulation of displacement and continuity conditions. This foundation sets the stage for presenting the computational implementation and the results obtained during this study. All implementations were performed in Python for MOC and Julia for GMC and HFGMC, with emphasis on modular, vectorized operations and data structures that facilitate direct extraction of subcell-level fields for machine learning applications.

E.2.1 Methodology

In the framework of the Method of Cells (MOC), Generalized Method of Cells (GMC), and High-Fidelity Generalized Method of Cells (HFGMC), the composite is modeled using a Representative Unit Cell (RUC) that captures the periodic microstructure. The RUC is partitioned into an array of rectangular subcells, as shown in Figure E.1, each assigned to either the fiber or matrix material. Below, the core formulations for each method are presented, followed by a discussion of their key differences in terms of displacement fields, continuity enforcement, and effective property computation.

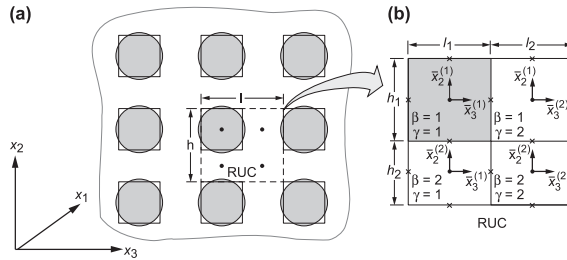


Figure E.1. MOC model of a continuously reinforced fiber composite. (a) A composite with a doubly periodic array of fibers extending in the x_1 -direction. (b) A repeating unit cell with four subcells ($\beta, \gamma = 1, 2$). Adapted from [174].

E.2.2 Method of Cells (MOC)

For MOC, the displacement field within each subcell is assumed to vary linearly with spatial coordinates:

$$u_i^{(\beta\gamma)}(x_1, x_2) = w_i^{(\beta\gamma)} + \phi_i^{(\beta\gamma)} x_1 + \theta_i^{(\beta\gamma)} x_2, \quad (\text{E.1})$$

where $u_i^{(\beta\gamma)}$ is the displacement component in the i -th direction for subcell (β, γ) , $w_i^{(\beta\gamma)}$ is the average displacement, and $\phi_i^{(\beta\gamma)}, \theta_i^{(\beta\gamma)}$ are displacement gradients in the x_1 and x_2 directions, respectively. Continuity between adjacent subcells is enforced in an average sense, ensuring displacement and traction compatibility over shared interfaces. The effective stress is computed by volume averaging:

$$\bar{\sigma}_{ij} = \frac{1}{V_{\text{RUC}}} \sum_{\beta, \gamma} \sigma_{ij}^{(\beta\gamma)} V^{(\beta\gamma)}, \quad (\text{E.2})$$

where $\sigma_{ij}^{(\beta\gamma)}$ and $V^{(\beta\gamma)}$ are the stress and volume of subcell (β, γ) , and V_{RUC} is the total RUC volume. This formulation yields closed-form solutions, prioritizing computational efficiency.

E.2.3 Generalized Method of Cells (GMC)

GMC extends MOC by refining the displacement field and continuity conditions. The displacement in each subcell remains linear, as in Equation (E.1), but is coupled through point-wise continuity of displacements and tractions at subcell interfaces:

$$u_i^{(\beta, \gamma)}(x_2 = h_\beta/2) = u_i^{(\beta+1, \gamma)}(x_2 = -h_{\beta+1}/2), \quad (\text{E.3})$$

and similarly for traction components $\sigma_{ij}^{(\beta, \gamma)} n_j$. The effective stress is computed as in Equation (E.2), but the point-wise continuity results in a larger system of equations solved numerically, allowing GMC to capture non-uniform strain fields within subcells.

E.2.4 High-Fidelity Generalized Method of Cells (HFGMC)

HFGMC further enhances the formulation by introducing a higher-order displacement field within each subcell:

$$u_i^{(\beta\gamma)}(x_1, x_2) = w_i^{(\beta\gamma)} + \phi_i^{(\beta\gamma)} x_1 + \theta_i^{(\beta\gamma)} x_2 + \sum_{m, n=2}^M \psi_{i(mn)}^{(\beta\gamma)} x_1^m x_2^n, \quad (\text{E.4})$$

where $\psi_{i(mn)}^{(\beta\gamma)}$ are coefficients of higher-order (typically quadratic, $M = 2$) polynomial terms. Continuity of displacements and tractions at subcell interfaces is enforced in an average integral sense, as in Equation (E.3) but integrated over interfaces. The effective stress follows Equation (E.2). The higher-order terms enable HFGMC to capture local stress and strain gradients with greater precision, at the cost of increased computational complexity.

E.2.5 Differences Between MOC, GMC, and HFGMC

The MOC, GMC, and HFGMC form a hierarchy of micromechanical models, each balancing accuracy and computational efficiency differently. MOC, the simplest of the three, assumes a linear displacement field, Equation (E.1), and enforces continuity in an average sense across subcell interfaces. This results in uniform stress and strain fields within each subcell, enabling closed-form solutions that are computationally efficient but less accurate for complex stress states or heterogeneous composites. The simplicity of MOC makes it ideal for rapid prototyping and generating preliminary datasets, as implemented in this study using Python for quick matrix operations.

GMC builds on MOC by maintaining the linear displacement field but enforcing point-wise continuity of displacements and tractions, Equation (E.3), at subcell interfaces. This allows GMC to capture non-uniform strain fields, improving accuracy for composites with significant phase contrasts or intricate microstructures. The trade-off is a larger system of equations requiring numerical solvers, which in this work was implemented using Julia to leverage its performance for matrix computations. GMC's richer local field data proved valuable for creating more detailed datasets suitable for machine learning applications.

HFGMC represents the most advanced method, incorporating higher-order displacement fields, Equation (E.4) to model local stress and strain gradients with high fidelity. It uses average integral continuity, but the polynomial terms increase the number of unknowns, significantly raising computational cost. In this study, HFGMC implementations required optimized Julia code to manage the larger computational load, producing highly detailed datasets that align well with machine learning requirements for capturing complex patterns. However, its complexity posed challenges for rapid dataset generation compared to MOC and GMC.

These differences guided the implementation choices in this work. MOC's simplicity facilitated initial code development and learning in Python, while GMC and HFGMC required advanced programming techniques in Julia to handle their numerical demands. The resulting datasets from each method varied in granularity, with MOC providing coarse but computationally efficient outputs, GMC offering a balance of detail and efficiency, and HFGMC delivering fine-grained data for potential machine learning applications, as explored in subsequent sections.

E.3 Sample Problem: Implementation of Micro-FGM in HFGMC

To extend the capabilities of the High-Fidelity Generalized Method of Cells (HFGMC), the original formulation was modified to allow each subcell to accommodate more than the conventional three material phases (matrix, fiber, and interphase). This extension enables the explicit modeling of micro-scale functionally graded materials (FGMs) within the interphase region of a Representative Unit Cell (RUC). In practice, this was

achieved by assigning graded material properties to consecutive subcells bridging the matrix and fiber, thereby creating a smooth transition in stiffness and strength. Such an implementation not only captures the effect of graded interphases on the overall response of composites, but also provides a flexible framework for generating diverse datasets suitable for machine learning applications. To demonstrate the potential of this modification, two representative RUC geometries were analyzed under loading conditions, and the results were evaluated in terms of stress contours, failure patterns, and stress-strain responses.

E.3.1 Material Library

Seven distinct material phases were defined to represent the matrix, fiber, and various interphase gradations. Their arbitrary properties are listed in Table E.1 and will be replaced with the actual values.

Table E.1. Material phases (arbitrary properties shown).

ID	Phase	E [GPa]	ν	Strength [MPa]
1	Matrix	3.50	0.35	90
2	Fiber	70.00	0.22	2500
3	Interphase lowest	3.85	0.25	99
4	Interphase low	4.20	0.25	108
5	Interphase mid	4.55	0.25	117
6	Interphase high	4.90	0.25	126
7	Interphase highest	5.25	0.25	135

E.3.2 Case Definitions

Five cases were designed to evaluate the influence of interphase modeling, ranging from simple matrix-fiber systems to graded and reverse-graded interphases. These are summarized in Table E.2.

Table E.2. Case definitions in terms of material phases.

Case	Description	Composition
A	Baseline composite	1, 2
B	With soft interphase	1, 2, 3
C	With stiff interphase	1, 2, 7
D	Graded interphase (soft $\rightarrow$ stiff)	1, 2, 3-7
E	Reverse graded (stiff $\rightarrow$ soft)	1, 2, 7-3

E.3.3 Geometry Definitions

Two representative RUC geometries were considered to evaluate the modified HFGMC code with multiple subcell materials. For simplicity, all subcells were assigned unit dimensions in both directions ($h = l = 1$), so that the RUC was discretized into a uniform grid of subcells. The material phases defined in Appendix E.3.1 were then assigned to subcells according to the cases (A–E). Color-coded schematics are provided to illustrate the material distributions.

- **Rectangular packing**

Rectangular packing consists of a rectangular RUC with 46×80 subcells. A central circular fiber of diameter 25 subcells is embedded within the matrix. Subcells inside the fiber are assigned the fiber material (2), the surrounding matrix subcells are assigned the matrix material (1), and interphase subcells (3–7) are placed between the fiber and the matrix according to the specific case configuration.

- **Hexagonal packing** Hexagonal packing extends rectangular one by adding four quarter-circle fibers at the corners of the RUC while retaining the central circular fiber. Material assignment follows the same convention as rectangular packing.

All five cases (A–E) described in Table E.2 were applied to both geometries. This setup allows systematic investigation of the effect of interphase grading and geometry complexity on stress distribution, failure patterns, and stress–strain responses.

E.3.4 Boundary Conditions

The boundary conditions were defined according to the RUC coordinate system shown in Figure E.1. A uniform global strain was applied in the x_2 -direction, while the x_1 - and x_3 -directions remained unconstrained, allowing free lateral deformation consistent with periodicity. Specifically, a total macroscopic strain of $\bar{\epsilon}_{22} = 0.05$ was imposed in the x_2 -direction. As in the classical GMC and its higher-order extensions, HFGMC, periodic boundary conditions were enforced on the opposite faces of the RUC. This ensures continuity of displacements and tractions across the boundaries, making the RUC representative of an infinite periodic microstructure. The applied global strain was thus translated into compatible boundary displacements at the subcell level, consistent with the HFGMC formulation.

E.3.5 Numerical Implementation

The HFGMC code was implemented in **Julia**, primarily for its performance advantages in handling large-scale matrix operations. The main computational bottleneck is the inversion of the system matrix, which was solved using Julia’s built-in backslash operator. This operator internally selects optimized factorization routines, e.g., LU or sparse solvers, ensuring numerical stability and efficiency without requiring explicit solver selection. The loading condition, defined in Appendix E.3.4, was applied incrementally in 1000 steps to capture the failure progression with sufficient resolution. At

each increment, subcell stresses were evaluated, and post-processing was conducted to assess local stress fields and detect failure. Failure analysis was based on the von Mises criterion, comparing the computed von Mises stress in each subcell against the material-specific ultimate strength provided in the material library, Table E.1. A failure margin was defined as:

$$\text{margin} = \sigma_{\text{ult}} - \sigma_{\text{vm}}, \quad (\text{E.5})$$

where σ_{ult} is the ultimate strength of the assigned material and σ_{vm} is the von Mises stress. Subcells were marked as failed when their margin became negative. To ensure robustness, a tolerance threshold was used when detecting new failures, as implemented in the custom function `EvalVonMises`. This framework allowed the generation of stress contours, stress-strain curves, and failure maps for all case studies, ensuring consistent evaluation across different material distributions and geometries.

E.4 Results

E.4.1 Stress-strain response

The macroscopic stress-strain curves obtained for the rectangular and hexagonal packings are presented in Figure E.2. A comparative analysis highlights the influence of interphase stiffness and grading direction on both stiffness and failure characteristics of the composites. For the rectangular packing, the introduction of a stiff interphase increases the initial slope of the stress-strain curve compared to the case without interphase. However, this configuration fails at lower strains and exhibits a distinct two-step degradation process: after the first failure event, the effective load-carrying capacity drops by roughly half, followed by a second reduction of similar magnitude, eventually leading to progressive damage without further stress increase. In contrast, the other interphase configurations maintain an initial slope nearly identical to the no-interphase case, but their failure modes differ. These cases undergo sudden, single-stage failure. Among them, the soft interphase shows the highest failure strain, followed by the stiff-to-soft graded interphase and then the soft-to-stiff one. Importantly, all interphase-containing cases reach higher ultimate strain levels compared to the composite without interphase.

In the hexagonal packing, the initial slopes of the curves are largely similar across the different cases. The soft interphase exhibits a slightly steeper initial slope but reaches failure earlier than all other cases. Failure in hexagonal arrangements is predominantly gradual, except for the no-interphase and stiff-interphase cases, which exhibit abrupt failure. The graded interphase cases (both stiff-to-soft and soft-to-stiff) display nearly overlapping stress-strain curves. They fail at stresses comparable to the stiff interphase case but with noticeably higher stiffness. Interestingly, while the stiff interphase has the lowest initial slope—close to that of the no-interphase case—it endures higher levels of stress and strain prior to final failure.

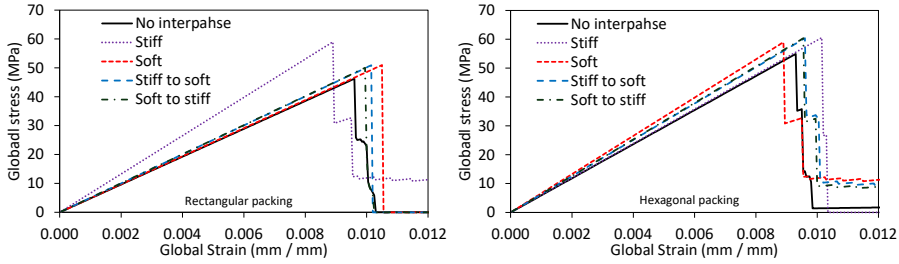


Figure E.2. Stress-strain curve for the studied HFGMC models.

E.4.2 Failure patterns: rectangular packing

To better understand the underlying damage mechanisms, the spatial distribution of failed subcells was examined at the initial and final loading stages. At zero strain, the figures serve as a reference, showing the geometry and material distribution within the representative unit cell. The color coding highlights the matrix, fiber, and interphase regions. At the final increment, the red subcells indicate failure according to the applied von Mises criterion.

Figure E.3 shows the geometrical and failure subcells for the rectangular packing. For the case without an interphase, the failure path develops tangentially to the fiber, producing a nearly linear crack trajectory along the matrix–fiber boundary. A similar trend is observed for the soft interphase configuration, where the crack propagates directly adjacent to the fiber surface. In contrast, when a stiff interphase is introduced, the crack trajectory shifts away from the fiber surface, developing between the fiber edge and the outer boundary of the interphase region. This separation zone may explain the increased slope of the stress–strain curve observed for this case.

In the graded interphase configurations, the crack paths are more sensitive to the grading direction. For the stiff-to-soft case, damage initiates in the subcells closest to the fiber–interphase boundary and then grows linearly outward. Conversely, in the soft-to-stiff case, failure originates within the softer region of the graded interphase and progresses into the matrix in a linear fashion. These distinct crack initiation sites underline the role of interphase grading in controlling failure evolution.

E.4.3 Failure patterns: hexagonal packing

Figure E.4 shows the geometrical and failure subcells for the rectangular packing. For the case without interphase, failure develops abruptly along paths tangential to the fiber, forming a sharp and continuous crack line. A similar sudden failure pattern is observed in the stiff interphase case, where the crack trajectory also aligns with the fiber perimeter but slightly penetrates into the matrix. In both cases, the damage localization results in a brittle-like response, consistent with the sudden stress drops observed in the stress–strain curves.

In contrast, the configurations with graded interphases display more distributed and gradual crack propagation. For both the soft-to-stiff and stiff-to-soft gradations, the damage initiates within the interphase region and extends smoothly into the surrounding matrix. This distributed failure mechanism results in a more progressive loss of stiffness, in agreement with the smoother decline observed in the macroscopic stress-strain response. The soft interphase case shows the most gradual damage evolution, with cracks initiating near the matrix-interphase boundary and spreading evenly across the interphase, thereby delaying complete failure.

Overall, the hexagonal packing promotes a more uniform stress distribution, which reduces the severity of localized damage compared to the rectangular configuration. The presence and type of interphase, particularly graded ones, play a critical role in determining not only the initiation site but also the progression of failure in this arrangement.

E.5 Conclusion

In this chapter, the High-Fidelity Generalized Method of Cells (HFGMC) was extended to allow multiple materials to be assigned to subcells, enabling the introduction of micro-functionally graded interphases within the representative unit cell. A systematic set of simulations was carried out for rectangular and hexagonal fiber packings, considering five cases of interphase design: no interphase, stiff interphase, soft interphase, soft-to-stiff graded interphase, and stiff-to-soft graded interphase. The results demonstrated that the presence and grading of the interphase significantly influence both the stress-strain response and the failure mechanisms. Rectangular packing tended to exhibit more abrupt failure modes, while hexagonal packing promoted smoother, progressive damage evolution. The graded interphases provided a balance between stiffness and toughness, leading to improved strain-to-failure compared to uniform interphases.

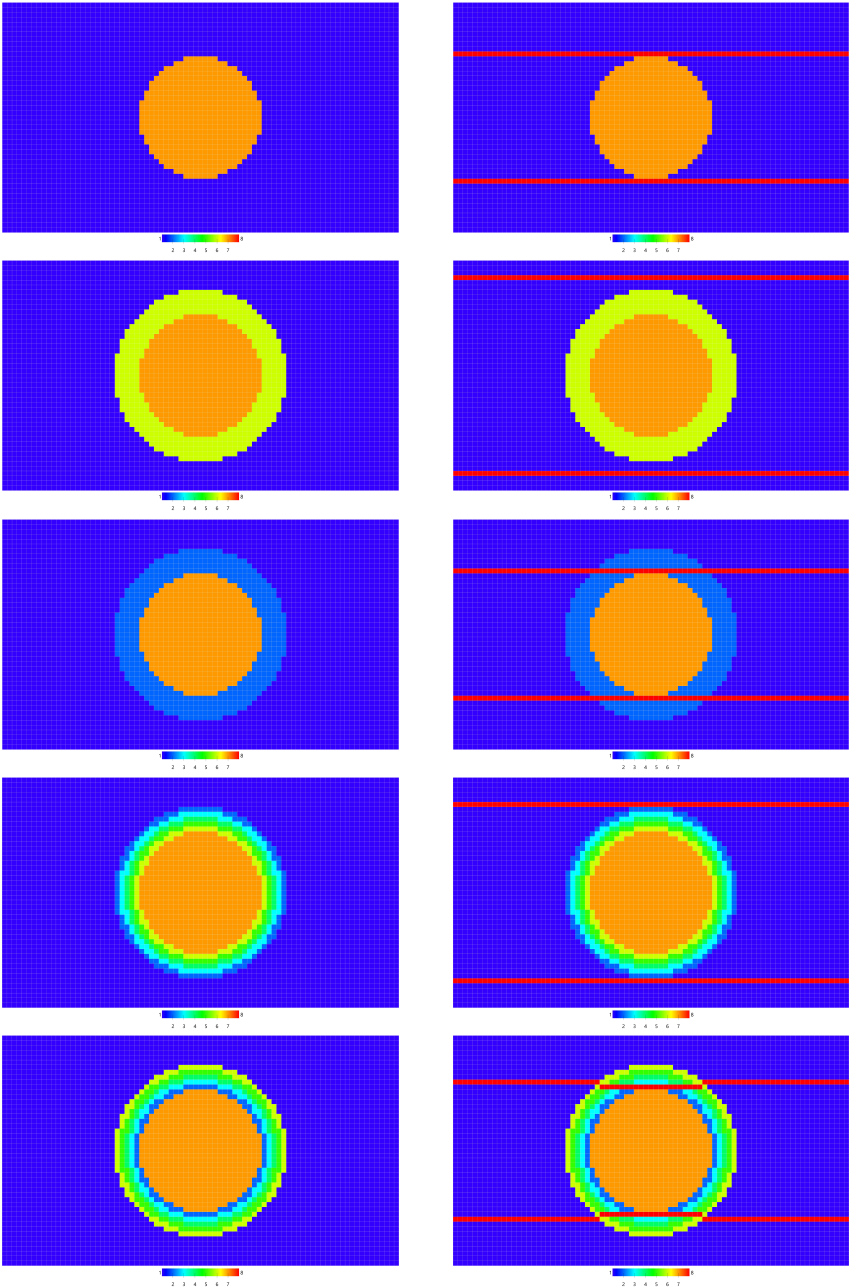


Figure E.3. Material distribution and failure pattern of the simulated HFGMC samples for the rectangular packing configuration.

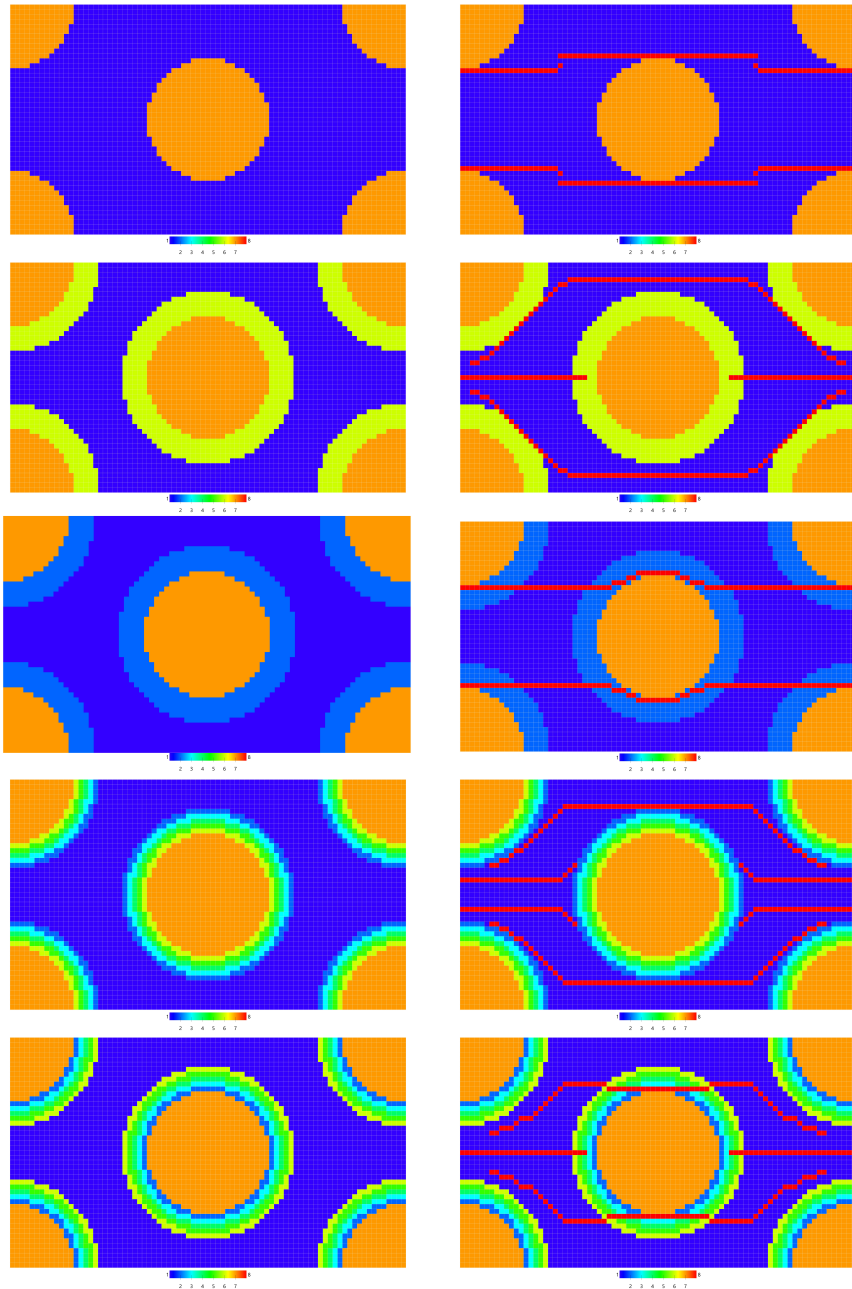


Figure E.4. Material distribution and failure pattern of the simulated HFGMC samples for the hexagonal packing configuration.

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