# Strategies for mechanical metamaterial design

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Chapter 1

# Introduction

## 1.1 Introduction

A branch of metamaterials [1–3], mechanical metamaterials are carefully engineered artificial structures prominent for their exotic and tunable mechanical properties, which are often not associated with the natural materials. These properties are governed by the macro-, micro- or nanoscale architecture and arrangement of the constituting unit cells, rather than directly by the (chemical) composition of the material. Often, these properties arise from the finite number of internal soft degrees-of-freedom in the system that govern the allowed deformations. In the last two decades, several surprising examples have been reported such as auxetic materials [4–6], materials with vanishing shear modulus [7, 8], materials with negative compressibility [9, 10], singularly nonlinear materials [11, 12], origami(-inspired) metamaterials [13–16], topological metamaterials [17–19], and multistable and programmable mechanical metamaterials [20] etc.

To a starter, the world of mechanical metamaterials can be best introduced by the help of examples that demonstrate which exotic properties and functionalities have been thus far realized. Below, we broadly categorize these featured properties and briefly mention some famous corresponding examples.

**Extremal materials** – Milton and Cherkaev theoretically proposed extremal materials in 1995 and defined them as materials that are extremely stiff in certain modes of deformation, while extremely compliant in the other modes [21]. Kadic et al. demonstrated that the theoretically possible pentamode metamaterials, which have extremely large bulk modulus compared to the shear modulus, can be realized experimentally by periodic placement of a specially designed artificial crystal, thereby pushing the boundaries for materials with exceptional response parameters [Fig. 1.1(a)] [7]. The solid lattice structure shears or deforms easily. At the same time the lattice is extremely hard to compress. These pentamode materials are therefore sometimes also called *metafluids*. Based on the pentamode metamaterials, Buckmann et al. later showed an experimental demonstration of a mechanical cloak [Fig. 1.1(b)] [8].

Another class of extremal materials are dilational materials, where the bulk modulus is extremely low and the shear modulus is extremely high. Several examples of dilational metamaterials can be found in the literature [22–25]. For these materials the Poisson's ratio, $\nu$ takes on the value -1. Any material with a negative value of $\nu$ is called an *auxetic* material. An archetypal example would be a quasi-2D elastic slab pierced with circular holes on a square array [26, 27]. Upon compression, the elastic slab undergoes buckling at the connector ligaments and attains a state of mutually orthogonal ellipses [Fig. 1.1(c)]. This pattern transformation allows the sample to exhibit a negative value of the Poisson's ratio.

**Shape Morphing and Multistability** – Tunability in the response properties is a common theme in the area of metamaterial research, which includes optical and electromagnetic counterparts as well [28–31]. The reconfigurable design of mechanical metamaterials is aimed to do just that by allowing for multiple switchable states, which usually occur by the reconfiguration of the lattice or unit cell geometry. The most striking examples are rigid folding based origami metamaterials, in which the faces between the creases remain rigid during folding/unfolding and only the creases bend [32]. The most studied one is the Miura-ori and its derivative crease patterns [13, 14, 33]. Waitukaitis et al. demonstrated that the simplest building blocks of origami, the degree-4 vertices, can be multistable with upto six possible stable states. Further, these 4-vertices can be tiled periodically into large tessellations allowing to create multistable *metasheets* that can be externally actuated to morph from one state to another [Fig. 1.1(d)] [34]. Departing away from strict rigid folding, Pinson et al. presented

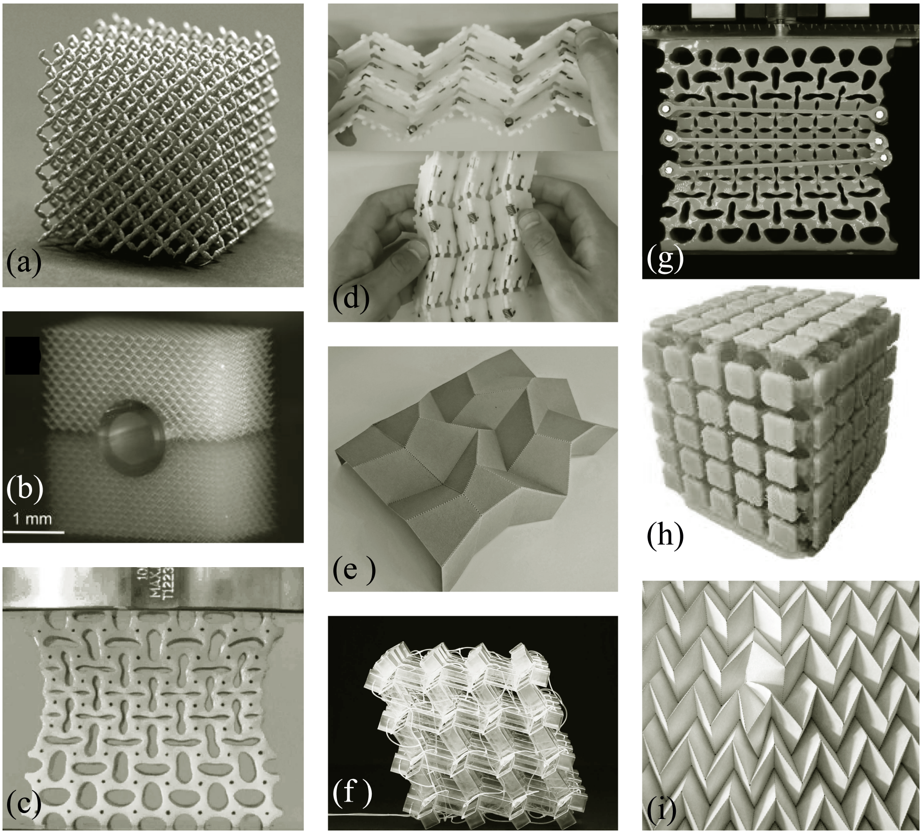


**Figure 1.1:** A gallery of some of the famous examples of mechanical metamaterials that demonstrate key concepts such as exceptional material response, shape morphability and programmability in the mechanical response. (a) pentamode metamaterials that are easy to shear but hard to compress [7], (b) a mechanical cloak based on pentamode metamaterials [8], (c) an auxetic material with a negative value of the Poisson's ratio [26], (d) rigid folding based multistable origami *metasheets* [34], (e) computer-designed novel foldable origami patterns that do not feature strict rigid folding [35], (f) an origami-inspired shape-transformable mechanical metamaterial [16], (g) a programmable mechanical metamaterial that exhibits programmability in the mechanical response [20], (h) a 3D mechanical metamaterial whose inner comprising unit cells can be stacked combinatorially to achieve diverse shape-shifting behavior [37], (i) a miura-ori origami pattern with local pop-through defects that control the compressive modulus of the overall structure [13]. Images are adopted from the respective cited sources.

a systematical approach to sample arbitrary origami crease patterns based on their folding energy and reported numerous near-perfect origami mechanisms, which can be deployed in situations where accidental self-folding needs to be avoided [Fig. 1.1(e)] [35]. Shape morphing and multistability are widespread in other categories of mechanical metamaterials as well. Rafsanjani et al. reported a class of switchable networks consisting of rigid rotating units connected with complaint hinges that simultaneously exhibit auxeticity and structural bistability [36].

**Programmability –** The essence of mechanical metamaterials is to let the structural design determine the mechanical response. Florijn et al. showed that if in the sample shown in Fig. 1.1(c), the alternate holes are made unequal in size [Fig. 1.1(g)], the sample retains the buckling induced auxeticity, albeit the buckled state is now dependent along which primary axis the sample is compressed. The precise tuning of these two decoupled deformations allowed to achieve programmability in the mechanical response [20]. Moving ahead from planar elastic metamaterials towards 3D shapes, Coulais et al. reported a class of aperiodic yet frustration-free architectures designed combinatorially using special cubic unit cells - *voxels* - such that their collective deformations can result in a shape morphing behavior, which can be preprogrammed due to multiple combinatorial possibilities in the arrangement of these voxels [Fig. 1.1(h)] [37]. Silverberg et al. demonstrated programmability in the mechanical response of the Miura-ori origami tessellation. There it was show that the mechanically bi-stable internal unit cells can be 'switched on' to act as local defects analogous to a crystal lattice and thus helping in tune the compressive modulus of the sheet [Fig. 1.1(i)] [13].

The examples of mechanical metamaterials cited above mainly deform by exploiting frustration-free low energy deformation pathways in the structure [37]. Very often its is possible to imitate the desired deformation mode by the free motion mode of an idealized mechanism consisting of hinging/rotating rigid geometrical parts [18, 38–41]. As a matter of fact, these mechanisms serve as an intuitive starting point to initiate and adapt the design to the requirements [20, 42]. Soft mechanical metamaterials can then be fabricated by joining stiffer elements with flexible, slender hinges allowing to achieve large deformations. Intuition based strategies to design mechanical metamaterials bottom-up from their base mechanisms can lead to a couple of general limitations: *(i)* the designs can be generic and periodic, *(ii)* materials exhibiting simpler functionalities are simple to discover and vice-versa. These limitations can be mitigated by adopting inverse methods for material design, which we discuss in the details below.

## 1.2 Inverse Strategies for Material Design

Across wide areas, inverse strategies are emerging as a promising approach in the realm of rationally designing the materials with desired properties [43–51]. The central idea is to come up with a framework which takes functional requirements as input and delivers the macroscopic design of the structure that satisfies them as output. Following such a strategy possesses several advantages over traditional engineering methods for material design. In the absence of some physical theory that connects the response function of the material with its structural design, the usual method to optimize the former is via tweaking the later, followed by synthesizing and testing. This approach is severely limited as only the simpler tasks can be easily handled. For complex tasks, one usually is content with very suboptimal designs, and not to mention that the traditional methods can be very time consuming.

Significant improvements in the computational capabilities and state-of-the-art fabrication techniques such as 3D printing (to fabricate complex designs intricately) in recent times have led to new advancements towards more logical inverse methods, which have been in practice since much earlier [52, 53]. These methods allow to handle complex design tasks and the whole process can be fully automated too, allowing to design materials on demand with varying target properties [54]. Another major benefit of deploying such techniques is that they typically result in the discovery of many near-perfect designs that fit the target criteria *quite closely*, thus significantly enlarging the design space and enabling its systematic explorations, which further aids in gaining a better understanding of the design space [35].

One way to carry out the design is by following an optimization-based methodology. In here, the main task of finding the optimal material design is formulated as an optimization problem, to do which, one has to first identify the shape parameters of the design that control the target response - *design variables.* The next step is to construct a physical or numerical model that simulates the material functioning on a computer, and is able to estimate the quality of any valid arbitrary design. The formal terminology

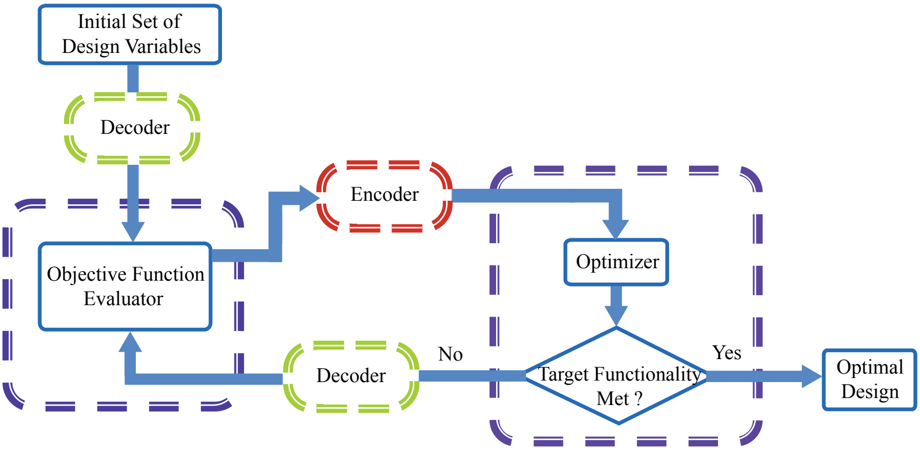
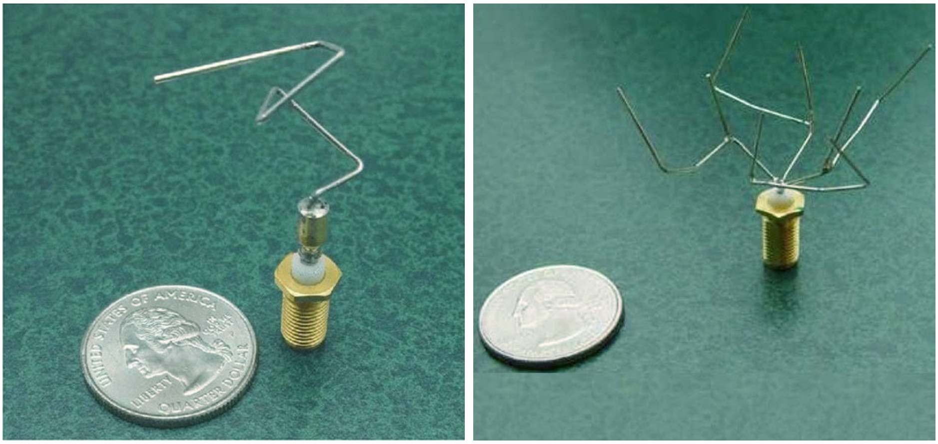


**Figure 1.2:** An optimization-based automated material design framework, that renders optimal design to match a given target property. Starting from an initial set of design variables, the optimizer searches for the optimal values of the design variables such that the objective function, which is a function of design variables, is maximized or minimized. Depending upon the implementation of the optimization algorithm, often the interfacing between the optimizer and the objective function evaluator consists of an intermediate encoding-decoding step that involves the mapping between coding space and the design space [55].

for this is *objective function* value which in effect is controlled by the values of design variables. The objective function measures the quality or *fitness* of a candidate design (solution). For example, if a minimization problem is formulated, low objective function values would correspond to better quality of design. With this framework, one is now set to optimize the design variables for the desired target behavior.

Complexity of a design optimization problem is dependent upon the dimensionality, which in turn is given by the total number of design variables. Higher dimensionality implies a very likely complex objective function landscape consisting of several local minima. This leads to an ineffectiveness of using gradient-based methods [56]. A far more promising choice in such cases is to use nature-inspired search heuristics that use a population-based method to efficiently explore the search space; think of genetic algorithms, evolutionary strategies, swarm intelligence algorithms, genetic programming



**(a)** **(b)**

**Figure 1.3:** Prototype photographs of evolved antenna designed by NASA for their Space Technology 5 (ST5) mission with set specific requirements for two desired radiation patterns: antenna's named (a) ST5-33-142-7 and (b) ST5-3-10 [63]. Images are adopted from the main source.

etc. [57–62]. The purpose of these algorithms is to optimize the values of design variables such that the target criteria is met. An objective function evaluator and an optimizer can together interface to form an automated design framework that takes a target material functionality as input and renders the optimal structural design as output. The process is schematically shown in Fig. 1.2.

In past, the employment of evolutionary (and related) search algorithms for design optimization purposes has delivered promising results across diverse fields such as in aerodynamics [53], structural engineering [64], design of mechanical components [51, 65], robotics [66, 67], Lithium-ion battery design [68], crystal structure prediction [47] and many more. We show in Fig. 1.3, *evolved antenna* designs reported by NASA in 2006, where evolutionary algorithms were utilized to discover sophisticated designs for prescribed radiation patterns of the antenna [63].

In this thesis, we present novel inverse strategies to design 2D mechanical metamaterials, whose internal deformations can be captured by underlying idealized mechanisms consisting of hinging rigid parts. We show that by optimizing for the characteristic trajectory of these single degree-of-freedom mechanisms, one can design generic metamaterials that exhibit complex mechanics, atypical zero-energy deformations and shape-transformable behavior.

## 1.3 Outline of the Thesis

The second chapter of this thesis serves as a inspiration as to what level of insights can be obtained by modeling the deformation of a mechanical metamaterial by its base mechanism. Specifically, we discuss in details a physical approach to analytically model the experimentally observed different mechanical regimes of a laterally confined *biholar* mechanical metamaterial reported in [20]. We show that non only a simple one-degree-of-freedom mechanism - *soft mechanism* - consisting of pin-jointed rectangles qualitatively captures the mechanical trends, but - and as the most relevant result of the chapter - also, conversely provides with an inverse strategy to design mechanical metamaterials for many more complex confinement-controlled mechanical responses. We suggest that based on the trajectory of a mechanism, various complex bifurcation sequences can be encoded, which unfold as the control parameter (amount of horizontal confinement here) is varied. We then show that coupling the hinges of the soft mechanism with torsional springs models the ligament thickness well. Finally, we utilize the soft mechanism to probe the limiting case, where the neighboring holes of the biholar sheet approach to be of equal size, and mathematically show that these regimes emerge from the unfolding of an imperfect pitchfork bifurcation.

In the third chapter of this thesis, we demonstrate a nature-inspired search strategy to design the optimal geometry of 2D unit cells that are not periodic but can still allow for atypical (approximate) zero-energy modes. We pursue it by the design of its underling mechanism. We begin with a single degree-of-freedom *precursor mechanism* consisting of pin-jointed polygons, whose internal motion can be captured by a characteristic curve. We then optimize the geometrical design of the mechanism such that the curve encoding the internal motion matches a prescribed target curve. We show that via this strategy, our search algorithm is able to discover plethora of *pseudo-mechanisms* with a very soft deformation mode that are far away from a true mechanism with a strict zero-energy mode. Further, we investigate the functioning of our algorithm and characterize it to gain insights into its search quality, solution distribution and exploration behavior of the search space. We then demonstrate a simple but elegant method to tile these unit cells into regular tessellations - *metatilings*, while still preserving the original soft more. Finally, we bring these unit cells and metatilings to life via 3D printing and confirm the expected deformation modes experimentally.

In the fourth chapter of this thesis, we demonstrate a crucial capability of an automated material design framework, which is the ability to optimize the structural shape for not just one but for multiple target properties. We input different target curves into our model in order to: *(i)* quantify the functioning of our model versus the complexity of the design task (target curves), and *(ii)* design and fabricate 2D bi-stable and tri-stable unit cells consisting of rigid units connected together through flexible slender linkages. Finally, we show that by carefully harnessing the elastic-frustration, one can tessellate copies of these unit cells and obtain larger shape-transforming mechanical metamaterials.