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UNIVERSITY OF CALIFORNIA SAN DIEGO

Design of material nonlinearity via topology optimization for applications in wave tailoring

A dissertation submitted in partial satisfaction of the
requirements for the degree Doctor of Philosophy

in

Engineering Sciences (Aerospace Engineering)

by

Brianna MacNider

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2024

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University of California San Diego

2024

DEDICATION

For Mom, forever and always my biggest and most dedicated supporter. I appreciate you more than words can say.

And for Dad, who did not get to see me enter this stage of my life, but who would, I think, have been very proud.

EPIGRAPH

I may not have gone where I intended to go, but I think I have ended up where I needed to be. -
Douglas Adams

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ABSTRACT OF THE DISSERTATION

Design of material nonlinearity via topology optimization for applications in wave tailoring

by

Brianna MacNider

Doctor of Philosophy in Engineering Sciences (Aerospace Engineering)

University of California San Diego, 2024

Nicholas Boechler, Chair

The use of architecture built into materials has led to the development of mechanical and acoustic metamaterials, which have enabled extraordinary and unprecedented manipulation of material properties (both static and dynamic). Despite this progress, significant challenges remain for metamaterial design, particularly as concerns highly nonlinear and high strain rate regimes. Herein, we focus on three challenges within this scope: inverse design of the mesostructured for nonlinear mechanical response, incorporating nonlinear wave effects into the inverse design, and

the influence of high strain rate effects on the modeling and design of such materials. A deep dive into these challenges is undertaken, exploring each of them in more detail. Both modeling and experiments are used to make strides in addressing the challenges of inverse design for nonlinear wave tailoring, in which a nonlinear inverse design framework coupled with a reduced order discrete element model is proposed and implemented. Experimental work is then undertaken to more thoroughly explore the challenges posed by high strain rates. Through these efforts, this work advances toward the goal of inversely designed high strain rate nonlinear metamaterials.

Chapter 1

Introduction

1.1 Motivation

Since the dawn of civilization humankind has sought to control its surroundings and master its environment through the manipulation of materials. The influence of material technology on the progression of human civilization has been so great that entire ages of history are named for the materials used to forge them - stone, copper, bronze, and iron. As greater and more precise control has been gained over material refining, processing, and manufacturing, the materials we use have been increasingly tailored to suit the needs of their intended function. These adjustments have largely been achieved by taking advantage of the already existent properties of the materials at play, exploiting the ever deepening knowledge of chemistry, physics, and material properties. In more recent years, there have been investigations into materials which utilize the intentional incorporation of lower-scale structures to effect the properties of the macroscale material. The manipulation of this lower scale structure has the potential to unlock advanced, precise tailoring of materials through clever design of the mesoscale structure, achieving properties that go beyond those seen in conventional materials. Herein lies the next grand frontier - designer materials, precisely customized for their applications through the manipulation of incorporated structure.

These structured materials, commonly referred to as architected materials, cellular materials, or lattice materials, rely upon sub-bulk structure to modify the property of the bulk material, achieving a separation of scales while allowing the lower scale structure to contribute

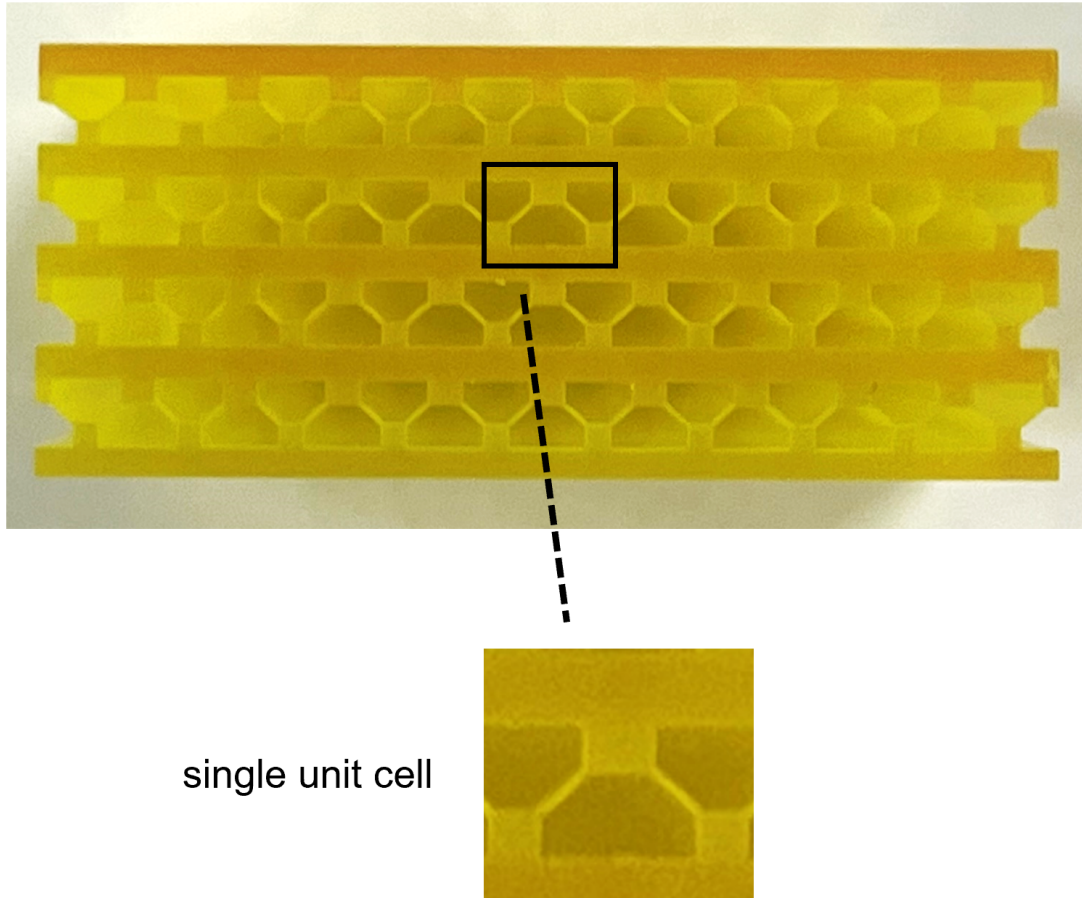


Figure 1.1. A 3D printed architected material composed of repeating units which consist of two slender (bistable) beams, with the incorporated structure of a single unit cell highlighted.

to the macroscale properties of the material. Architected materials are found extensively in nature in structures such as wood, bone, beaks, and honeycombs, as well as in foams [1]. As the properties of the bulk material are largely dependent on the geometry of the mesostructure, instead of only the constituent material properties, there exists the potential for a great degree of tailorability through manipulation of said geometry. Through variation of the architecture, the material scale properties can be tailored to optimize the desired functionality. With the advent of additive manufacturing, realizing the intentional design and construction of the mesoscale geometry on length scales that can be useful has become easier than ever to achieve [2].

This has led to a renaissance of architected lattice designs for a wide array of applications. The incorporation of mesoscale structure can lead to superior properties and lowered weight,

and has been found to have useful applications in stiff lightweight structures, impact mitigation, vibration damping, thermal insulation, and acoustic absorption [1, 3]. Furthermore, designed mesostructures can be used to achieve properties not usually found in nature, in which case they can be classified as metamaterials [4, 5]. Metamaterials (a subclass of architected materials) have a broad range of definitions, but can be thought of as materials which achieve properties outside of those generally seen in natural materials through the use of mesoscale structure, often in the context of wave manipulation (in which case the mesoscale structure is sub-wavelength). The first research efforts into metamaterials focused on the manipulation of electromagnetic waves, using the mesostructure to achieve phenomenon such as negative refractive indices and cloaking [6]. Of particular interest herein, however, is the expansion of these ideas into their mechanical counterparts; acoustic and mechanical metamaterials. These metamaterials utilize the mesostructure to manipulate acoustic waves, rather than electromagnetic ones [7], as well as to achieve extreme static properties [5]. This has led to dynamic functionalities such as acoustic cloaking, zero or negative refractive index, and asymmetric energy transfer [4, 8], and quasi-static functionalities such as negative properties (including Poisson's ratio and stiffness), and designs for applications in energy harvesting, vibration control, sensing, and actuation [5]. Research into new metamaterial designs and functionalities is progressing at a rapid rate, highlighting the great promise these materials show as they continue to mature.

While metamaterials can utilize active elements, there is particular promise in passive metamaterials, which achieve their extraordinary properties through the use of the mesostructure geometry alone. An ideal end objective would be the ability to precisely tailor the mesostructure of such materials for a desired application. Simply tailoring quasi-static behavior is a piece of the puzzle, but not the entire puzzle, as applications in dynamics and wave tailoring are greatly desired. The inclusion of wave effects is attractive in that it introduces phenomenon such as dispersion and band gaps, with direct applications in signal processing and vibration control. Furthermore, introducing nonlinear waves gives rise to still more unique and promising phenomenon such as solitons, breathers, kinks, etc. [9]. Beyond acoustic wave tailoring, however,

there is significant interest in applications at higher strain rates such as ballistic impact, shock loading, and explosives. These loading scenarios produce strain rates on the order of $\sim 10^3 \text{ s}^{-1}$ or higher, and applications dealing with protective materials and impact mitigation therefore must operate within this regime. Yet, despite the promise of structured materials, the application of tailored metamaterials to higher strain rate regimes has proved to be an exceptionally difficult challenge. The question of what challenges exist, and why they have yet to be overcome, is a critical one to address in the advancement of the tailoring of architected materials. We propose that these challenges can be roughly grouped into three main categories, as follows: 1) the inverse design of the mesostructure for targeted nonlinear response, 2) the incorporation of nonlinear wave effects (across length scales) into the inverse design, and 3) the incorporation of high strain rate effects (both intermediate and very high) into the modeling and inverse design. The next few paragraphs endeavor to give a broad context to these challenges.

Until recently, the design of architected materials has heavily relied on conveniently available or known structural unit cell elements, such as octet [10], different orientations of simple cubic [11], honeycomb [12], TPMS (triply periodic minimal surface) type structures [13], as well as modifications to these designs. Structures classified as passive metamaterials, meanwhile, have also made heavy use of easily available or known elements, such as trusses [14], snapping beams [15], Helmholtz resonators [16], rotating squares [17], and kirigami structures [18]. Despite the amazing things that have been done with these materials, extending their design to new and improved applications has remained difficult. They are tailorable in a broad sense, in that known unit cells can be rearranged in unique ways, modified slightly to produce new properties or adjust existing ones, and new and interesting elements can be incorporated as they are discovered - but in a specific sense, full tailorability of the mesostructure is still somewhat lacking. In order to truly unlock the potential of such materials, they need to be able to target specific purposes through highly precise design of the mesostructure, influencing the macroscale properties exactly as desired. At the level of control and applications of interest to us, this involves not just applying known mesostructural elements, but the incorporation

of intentionally designed, application specific nonlinearities into the mesostructure. However, designing a (meso)structure to achieve a specific, desired, intentional nonlinearity can be non-intuitive and difficult, unless the desired nonlinearity happens to fit into a known class or design. Even then, while broad tailoring (e.g. achieving a stiffening nonlinearity, or a snap-through type nonlinearity) is doable, precise tailoring of the nonlinearity is much more difficult. There have been some inverse design attempts at tailoring properties of structures such as targeted Poisson's ratio [19], maximized energy absorption [20], or targeted band gaps [21]. For many applications, however, the nonlinear properties of the available unit cells have not been continuously tailorable, limiting the available target functionalities at the material scale. In the last several years, advances in inverse design methods have enabled both broad and precise (*i.e.* able to achieve multiple types of nonlinear behavior, and able to do so well) tailoring of nonlinear constitutive behavior of a structure [22–24]. With this, the quasi-static behavior of unit cells can be customized for a desired nonlinear behavior, which can then be incorporated into a bulk, designer architected material.

Precisely customizable nonlinear materials for quasi-static effects has already proven to be a difficult goal to achieve, however, the inclusion of system-level wave effects only amplifies the complexity of the problem. Due to the separation of length scales in such a problem, one must simultaneously modify the sub-bulk unit cell design while also considering the dynamics at the system scale. The interplay between the nonlinearity of the constituent material, the geometry, and the relevant length scales quickly becomes a complex inverse design problem. While such simulations are doable with modern computing, they are often costly in terms of computation time and effort. Since inverse design approaches generally work in an iterative manner, converging toward desired behavior step by step, the computational cost to a full-fidelity inverse design across length scales can be prohibitive.

At relatively low strain rates, while the inverse design problem is complex, wave effects may be incorporated through consideration of the length scales involved via a coupling of different length scale models (described in more detail in the Background on Inverse Design

section below). This provides a reasonably accurate representative model of the problem. More intractable complications are added when one considers increasing the strain rate to regimes in which the quasi-static design principles no longer encompass the entirety of the relevant mechanisms. Material strain rate sensitivity (such as viscoelasticity) and inertial effects gain increasing importance as strain rates are increased. The loading scenario (strain rate and deformation) may drive onset of plasticity and failure modes, many of them strain rate sensitive (such as viscoelasticity associated brittle fracture). It is not yet clear how to easily encompass all of these components into an inverse design problem, as the required modeling is complex and computationally intensive, limiting the ability (even further) to iteratively optimize while also including all important physics. In pursuit of the eventual goal of enabling such inverse design attempts, it is imperative to understand the relevance of various strain-rate sensitive effects at diverse length scales and strain rate regimes. Experimental investigations into the response of materials at various strain rates, from intermediate up into the shock regime, can provide vital insight into this problem.

Given the extreme complexity and many challenges of the goal of inversely designing architected materials for high strain rate applications, we propose insight can be gained by breaking the problem down into smaller steps. This work therefore takes the approach of breaking it down into more manageable pieces to investigate - namely, the inverse design of nonlinearity into a mesostructure for wave tailoring purposes, and the further investigation of strain rate effects on the behavior of structures and materials, for eventual incorporation into the former. The following pages therefore include a more thorough review of the relevant background and literature in the fields of inverse design for nonlinear properties, the properties of architected materials and their strain rate sensitivity at intermediate strain rates, and higher strain rate shock physics.

1.2 Background on Inverse Design

Initial attempts at the design and fabrication of mechanical metamaterials relied upon knowledge of mechanics and the design space to make largely intuition-driven designs. Later designs have also aimed to incorporate tunability through the use of elements which can be adjusted by small amounts to achieve a shift in behavior. Examples include adjusting pre-stress to change the force-displacement response in tensegrity structures [25], using active magnetic fields to tune the stiffness of springs within a metamaterial [26], the use of lateral confinement to control buckling response [27], the use of notches in kirigami metamaterials [28], and introducing hybrid cut patterns to kirigami structures [29], to name but a few. Designing in this way can be limited in scope, however. Inverse design presents the potential for a much more efficient and effective way of discovering the mesostructure needed for a particular application.

Computational inverse design can be defined as a process wherein a desired functionality (the objective) is taken as an input, and a computational method is used to generate an output design which, ideally, displays functionality close to this target property within a set of imposed constraints. Common target objectives include high stiffness with low mass [30, 31], desired heat or fluid flow properties [32, 33], or targeted Poisson's ratio [19, 34]. A subset of inverse design methods includes topology optimization, a method by which the topology of a structure is parameterized such that it can be represented as a set of design variables, which can be differentiated to obtain sensitivity information for a gradient descent optimization. The problem is solved, generally via finite element method (FEM), which allows the calculation of the sensitivities and the update of the design variables. Topology optimization generally requires higher computation times relative to reduced order methods, due to the relatively large number of design variables and the need to solve the full FEM problem for each iteration of the optimization. Additionally, gradient descent methods can converge to a non-ideal objective due to the presence of local minima in the design space (which is particularly true for highly nonlinear problems). However, topology optimization has the advantage of being high fidelity, and able

to capture a wide array of physics with high accuracy due to the continuous representation of the design. Designs are also generally highly tailorable due to the large number of design variables, enabling closer matches to the objective than might be expected in some reduced order approaches. There exist a variety of topology optimization methods, which generally employ different approaches to the parameterization of the structure. These include, but are not limited to, solid isotropic material penalization (SIMP, which treats the density of each element as a design variable with a continuously variable density, with a penalization for intermediate densities) [35, 36], bidirectional evolutionary structural optimization (BESO, which removes and adds material in an iterative fashion where it is most efficient to do so) [37], and the level set method [38], which we will focus on here in greater detail.

The level set method defines an implicit function to separate the domains of full material and no material. This implicit function is taken to be a signed distance function representing the distance to the nearest boundary. In this parameterization, the boundary is represented as the zero level set, $\phi(x)$, such that

$$\begin{aligned}\phi(x) &\geq 0, & x \in \Omega \\ \phi(x) &= 0, & x \in \partial\Omega \\ \phi(x) &< 0, & x \ni \Omega\end{aligned}\tag{1.1}$$

,

where Ω is taken to be the structure, and $\partial\Omega$ is taken to be the boundary of the structure. This representation is highlighted in Fig. 1.2. In this approach, the locations of the boundary is treated as the design variable. Updates are calculated by considering a fictitious time, t , assuming that the structure evolves with some velocity $V(x, t)$, and then solving a Hamilton-Jacobi equation

$$\frac{\partial\phi}{\partial t} + V|\nabla\phi| = 0,\tag{1.2}$$

for the updates to the structure [38–41]. One of the great advantages of this approach is

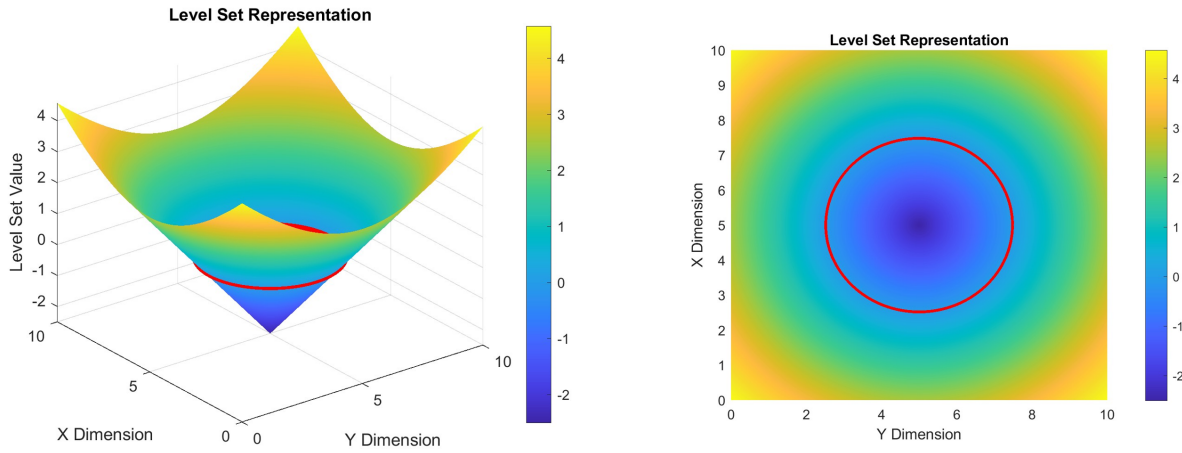


Figure 1.2. A representation of the level set method parameterization, with the zero level set highlighted in red. Negative values represent an absence of material, while positive values represent full material.

the inherently binary depiction of the design. Alternative topology optimization methods, such as density based methods, often encounter the problem of soft, intermediate elements, representing a state partially between full material and no material. These partial elements tend to blur the edges of the design, and allow designs that are difficult (if not impossible) to manufacture. Accordingly, various methods have been developed to minimize their presence, including penalizing intermediate elements in an attempt to gradually drive the design to a binary state (as is done in SIMP). The level set method, in contrast, avoids this issue through the representation of the structure boundary between two distinct domains, thus inherently achieving a binary representation. This method is therefore highly beneficial for use in problems in which high precision is desired or problems in which extra steps, such as the requirement to sharpen elements, may introduce additional complications to the design space.

The introduction of nonlinearity to the optimization process adds further complications to the modeling and solution processes. Nonlinear FEM and optimization methods which address these have been refined and developed over many years. First, it is helpful to define what is meant by a ‘nonlinear’ optimization. While there are several distinct forms of nonlinearity which can be introduced to an optimization problem, herein we focus on two main forms of

nonlinearity: material, and geometric. Material nonlinearity refers to nonlinearity introduced in the material constitutive model, the relationship between stress and strain. Geometric nonlinearity refers to nonlinearity introduced in the relationship between strain and displacement, often due to large deformation and rotations [42]. These two types of nonlinearity are often coupled, and often arise together in nonlinear problems. Nonetheless, geometric nonlinearity can exist independently of material nonlinearity. Implementation of nonlinear considerations requires the use of large deformation theory, which includes large deformation representations of the stress and strain tensors. Development of topology optimization methods incorporating geometric nonlinearity includes works focusing solely on geometric nonlinearity by [43, 44], as well as those incorporating both geometric and material nonlinearity [45, 46]. Early nonlinear and large deformation optimization methods were further developed in works which explored the inverse design of mechanisms and snap-through type behavior, including [47] and [48]. These nonlinear methods were further extended to level-set methods in the works of [41, 49].

The optimization of structures for targeted (often nonlinear) properties has proven to be a rich and varied research field. Examples include optimizations for properties such as Poisson’s ratio [19, 34, 50–52], maximized displacement (as in large deformation compliant mechanisms) [48, 53], stiffness and energy separations of mechanical logic gates [54], thermal expansion coefficients [55, 56], negative permeability in metamaterials [57], and many, many more. Achieving the targeted inverse design of a full nonlinear constitutive curve (*i.e.* characterized by multiple points along the curve such that the shape is accurately represented, rather than by few and very discrete points) in a continuous, 2D structure took further years to achieve. Early attempts included optimizing for one to two points along a nonlinear force-displacement curve in the pursuit of snap-through or mechanism-type behavior, often targeting specific limit points as snapping criteria [47, 48], and later similar attempts for specific applications such as bistable stents or morphing wing structures [58, 59]. Still further works took the approach of simplifying the problem in order to achieve fully tailorable nonlinear constitutive behavior, such as by representing nonlinear springs as splines [60, 61], or considering networks of trusses [34]. In the last

several years, advancements in computational resources and optimization techniques have at last led to the development of several methods capable of fully tailoring nonlinear force-displacement curves. Li et al. employ a two-material, SIMP based topology optimization method which has been shown to be capable of designing for stiffening, softening, bistable, and plateau-like nonlinearities [22, 62]. Still other recent works have leveraged advancements in data driven design to employ machine learning based inverse design methods for these problems. Deng et al. couple a genetic algorithm (GA) optimization approach with a reduced order model trained neural network to successfully design structures for a variety of softening and negative stiffness nonlinearities [23]. Chai et al. incorporate two neural networks to inversely design sheets of snapping structures [63]. Bastek and Kochmann make use of a video denoising diffusion approach, which uses simulated stresses and displacements to train a model capable of generating designs for a variety of nonlinearities not included within the training data set [64]. Ha et al. use generative machine learning incorporating both prediction and validation components to tailor the compressive behavior of lattice materials [65]. It should be noted, however, that these works employ quasi-static modeling of the designed structures (and, thus, do not incorporate dynamics or strain rate considerations), and are not necessarily designed to integrate well with explicit dynamics simulations.

Indeed, inverse design approaches undertaken with dynamic applications in mind have often not explicitly included consideration of dynamic behavior or processes (i.e. wave effects). For example, optimization approaches for impact mitigation often focus on increasing the energy encompassed within a force-displacement curve [20, 66], targeting plateau-like behavior [67], or otherwise tailoring snap-through type curves. However, this is accomplished through consideration of the quasi-static response of the structure, leaving out material strain rate sensitivity, inertial effects, and wave effects. As an approximation, at relatively low strain rates and for thin structures compared to the wavelengths, this approach works well. This is because at low strain rates, material strain rate dependency can be considered negligible, or at least of low enough importance that optimization approaches can be expected to produce improved designs

despite neglecting them, and for thin structures compared to the wavelengths involved, wave effects to not dominate the system response. As strain rate increases or characteristic wavelengths decrease, however, these effects begin to gain enough dominance that they fundamentally alter the behavior of the system. At this point, they can no longer be neglected. Additionally, by neglecting wave effects, the entire rich space of wave phenomenon is also neglected.

It should be mentioned that there exists a notable exception to this statement of neglecting wave effects in inverse design works which aim to optimize for acoustic properties such as targeted band gaps, wave damping, or wave guiding [21, 68–70]. In general, such attempts utilize periodic boundary conditions and Bloch’s theorem in order to inversely design for a desired frequency space response. However, this representation is incapable of taking into account strain rate effects in the material. It also requires several limiting assumptions, including linearity, small displacement, and a periodic representation which excludes the ability to spatially vary a design or allow non-periodic wave solutions.

In pursuit of the explicit, nonlinear, spatially variable incorporation of wave effects at the system length scale, one can envision the usefulness of representing the different length scales of the problem in the most convenient way for the physics which must be considered at that scale. While the mesostructure length scale of an architected material necessitates high fidelity in order to accurately capture the intricacies of the geometry, the system length scale need not include quite so much detail. An analogy can be drawn between the system length scale of an architected material and spring-mass systems, in which the designed mesostructure unit cell can be thought of as having homogenized behavior represented as a type of idealized, massless nonlinear spring connecting layers of point masses. This type of approximation is frequently made in wave and vibration analysis for continuous systems [71]. Such an approximation can be considered valid when we can assume one dimensional loading, that the mass of the point masses is much larger than the mass of the nonlinear springs, and that the point masses are much stiffer than the nonlinear springs. The tendency for some structured architected materials to be organized into distinct rows of unit cells works well with this assumption, and spring-

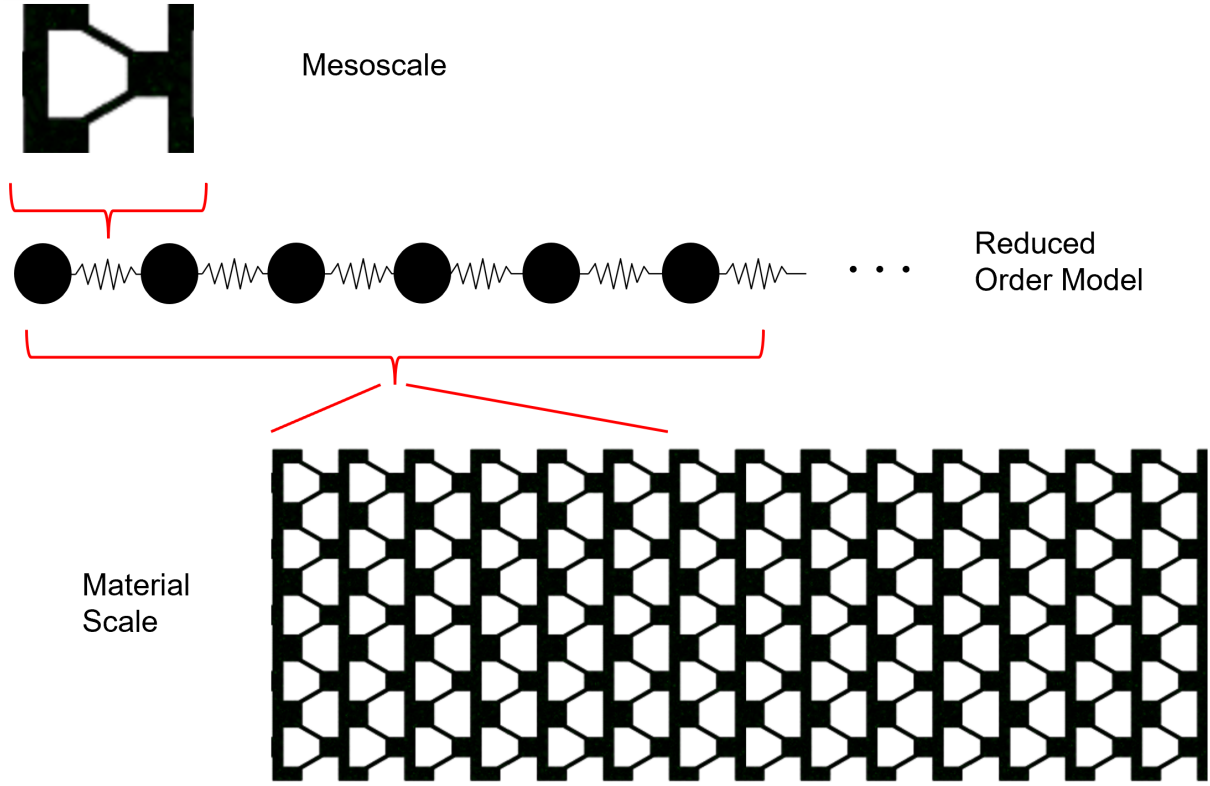


Figure 1.3. A representation of the separation of length scales allowing for the capturing of the relevant physics. The mesoscale is represented by the top row, the reduced order model capable of simulating wave transmission by the middle row, and the full fidelity material scale by the bottom row.

mass models have been used to represent architected materials extensively in literature [72, 73], including honeycombs [74] and foams [75]. This nonlinear spring can be furthermore thought of as a type of nonlinear constitutive law which could take one of any number of forms. In this context we propose it might conveniently be represented as some nonlinear polynomial of the form $F = c_1x + \sum_{i=1}^n c_i x^i$, in which i represents distinct nonlinear terms, and n represents the highest order of nonlinearity modeled. A reduced order spring-mass model of this form has the distinct advantage of being easily represented by a discrete element modeling approach, which in turn is a fast and computationally cheap system to simulate. Additionally, this representation is particularly useful in that a great deal of analytical dynamics and nonlinear wave explorations use spring-mass model representation [76].

1.3 Background on the Properties and Low-to-Intermediate Strain Rate Sensitivity of Architected Materials

As 3D printing technology has matured over the last several decades, structured architected materials have become an increasingly common focus of research. The high stiffness to weight ratio and excellent material properties of lattice materials has made them a popular choice for many applications. As interest in the applications of these materials has grown, so too has interest in applications at heightened strain rates, particular in the context of impact mitigation in regimes ranging from drop tests ($\sim 10^1 \text{ s}^{-1}$) to ballistic impacts $\sim 10^3 \text{ s}^{-1}$. Numerous studies, both computational and experimental, have been undertaken to investigate the performance of such structures under dynamic loading scenarios, as well as the influence of design and material parameters upon the performance.

To begin the discussion on the characterization of the strain rate response of architected materials, we first review several major important properties of such materials. Ashby described the now widely used distinction between two key types of cellular solids, those which are bending dominated and those which are stretching dominated [77]. The differentiation between the two classes can be made through the use of Maxwell's stability criterion, wherein counting the number of struts and joints informs if the structure acts as a mechanism (bending dominated, in the case of lattice structures), or not (stretch dominated) [77, 78]. Stretch dominated structures tend to be strong and lightweight, while bending dominated structures tend to give easily, but display long plateau regions in the force displacement curve, which is generally considered to be favorable for energy absorption. Also of interest in examining architected materials is the influence of relative density, given as

$$\frac{\rho}{\rho_s} = 1 - \varphi, \quad (1.3)$$

in which ρ is taken as the density of the structure, ρ_s is the density of the constituent material,

and ϕ is the porosity of the structure [3]. Generally, architected material compressive loading behavior begins with a linear elastic region of the force displacement curve, followed by some variation of negative stiffness, plateau, or yielding/plasticity (depending upon the material and geometry), and followed eventually by a region characterized by a sharp increase in stiffness once the densification strain is reached (that is, contact is made between the distinct geometric features of the mesostructure).

The most relevant parameters influencing the strain rate sensitive behavior of architected materials under dynamic loading include the strain rate sensitivity of the constituent material, the inertial effects (determined by the geometry of the mesostructure), and, potentially, the influence of trapped gas (in the case of closed-cell architected materials) [3, 79, 80]. We will neglect the discussion of trapped gas herein, as closed-cell materials are not a particular focus of this work.

The strain rate sensitivity of the constituent material is vital to the strain rate sensitivity of the overall structure. While the bulk strain rate sensitivity of many typical constituent materials (metals and polymers, typically) is a well studied topic [81, 82], the strain rate sensitivity applied to structured materials is not so straightforward. Firstly, we note that nonuniform deformation, arising from the influence of the geometry, often leads to stress concentrations and vastly different locally experienced strain rates within the mesostructure. Secondly, architected materials are increasingly being manufactured via additive manufacturing, which may introduce additional complications to the behavior of the bulk material due to the layer-by-layer nature of some methods. Experimental studies have been able to offer some insight as to the influence of the constituent material. It is well known that strain rate often stiffens or effectively strengthens bulk material, both in polymers [81] and metals [82]. This base material strain rate sensitivity has been shown to influence the strain rate sensitivity of the architected material [79, 83]. In addition, works examining high strain rate dynamic loading of architected materials with ductile constituent material often observe 'shock enhancement of compressive strength', or a 'Dynamic Increase Factor'. This effect raises the yield strength of the structure and can be thought of as arising from a type of 'shock front' of densifying cells in architected materials, and depends upon

both the initial properties and the velocity [83]. A simplified shock enhancement model was proposed by Reid and Peng to describe this observed behavior in wood, which has been shown to have some success at describing this phenomenon [84, 85]. Dynamic increase in strength has been noted experimentally in metallic honeycombs [86, 87], steel octet truss lattices [88], steel TPMS lattices [89, 90], and polymeric truss lattices [91], to name but a few. Conversely, it has also been found in some cases that increasing strain rate lowered the compressive strength, potentially due to the influence of thermal softening of the constituent material [92].

Non-ductile constituent material structures, on the other hand, encounter issues of increased brittleness and fracture at elevated strain rates. Many polymers, for example, have been shown to become brittle under dynamic loading scenarios, due in large part to the relative time scales of loading and relaxation times in the polymer [81, 93]. Accordingly, architected materials constructed from such base materials have been shown to fail catastrophically in fracture under impact [91, 94]. The choice of the constituent material, and the influence of its strain rate sensitivity, is therefore of great importance in the dynamic behavior of structured materials.

Inertia effects in architected materials have sometimes been categorized into macro- and micro- inertia effects [83, 85, 95]. Macro-inertia can be thought of as the inertia due to the motion of the center of mass of a representative volume element (RVE). Micro-inertia, meanwhile, is associated with the motion of individual mesostructure geometric features, such as cell walls, and is highly dependent upon the mesostructure geometry [79, 96, 97]. This may additionally be thought of in the context of Cosserat (or micropolar) media, in which a structured continuum can be modeled as a collection of particles which possess translational and rotational degrees of freedom, and therefore having an associated inertia [98].

Within this context, the work of Calladine and English is of relevance, in which the effects of inertia in two distinct types of structures, classified as Type I and Type II, were examined [96]. Type I structures can be thought of as those with a force-displacement profile consisting of a linear behavior followed by a plateau-like or slowly increasing region, while Type II can be classified as structures exhibiting a linear behavior followed by a sharp drop or region of negative

stiffness. It was found that Type II structures were significantly more strain rate sensitive. This sensitivity is associated with the shape of the quasi-static energy-deflection curve, which is in turn dependent entirely upon the geometry. The strain rate sensitivity in this case is analytically shown to stem from the increased inertia factor associated with high transverse accelerations in the angled beams in the Type II structure. Although not explicitly outlined in the relationship of Type I and Type II structures, the phenomenon of dynamic buckling is related to the observed strain rate sensitivity in Type II structures. When the mesostructure geometry is such that there is the potential for buckling of struts or cell walls to occur, elevated strain rates have the potential to qualitatively shift the buckling deformation mode due to the influence of inertia, resulting in a dynamic buckling mode. In such a scenario inertial effects can stabilize the buckling of a strut, preventing the onset of buckling and allowing for greater axial deformation and load support. This shifts the yield point of the structural response, effectively ‘strengthening’ the structure under dynamic loading [99–101]. For more complex geometries than the relatively simple one examined in Calladine and English, it is clear that similar types of energy-deflection curves produce inertia driven strain rate sensitivity, but the extent and interplay with material effects is less clear. This lack of clarity is exemplified by conflicting studies regarding the influence of inertia on the strain rate sensitivity of architected materials, with multiple works finding strain rate sensitivity stemming exclusively from the material response [88–90, 102], while multiple others find significant inertial effects [103–105], despite similar materials and strain rates in many cases. Still others have explicitly found that the inertia associated with the buckling of truss struts a significant and strain rate dependent effect in certain architected materials, such as pyramidal truss cores [106].

Of additional interest herein are dynamic loading regimes approaching the scenario in which force balance (equilibrium) is not maintained due to wave propagation, which can be taken as an indicator of macro-inertia effects [95]. Some works refer to this as a type of ‘shock’ regime due to the discontinuity across the propagating wave front, in which there is a sharp rise in stress and strain. It is important to distinguish this from very high strain rate shock regimes

characterized by complete crushing of the structure, and the differentiation is sometimes made between structural or ‘non-compaction’ shock (in architected materials at lower strain rates) and ‘compaction’ shock (higher strain rates, discussed further in the next section). At low strain rates the collapse of the mesostructure is generally random across the length of the sample, occurring at defects or weak points within the structure. At a sufficiently high loading rate, however, the collapse mode shifts to a sequential collapse of layers from the loading end in the direction of the loading pulse, as depicted in Fig. 1.4. This has been observed both experimentally [107] and computationally [104]. Additionally, some studies have shown the emergence of more complex modes than simple sequential collapse as a function of geometry and strain rate, such as ‘x’ and ‘v’ shaped bands [92, 108, 109]. The strain rate at which this transition of deformation mode occurs has been a subject of some investigation, and results have varied due to the complex interplay between dependence upon the geometry, the constituent material, and the length scales involved.

1.4 Background on Shock

At extreme strain rates, on the order of $\sim 10^4 - 10^6 \text{ s}^{-1}$, a qualitatively distinct regime characterized by sharp pressure discontinuities, or shock, is entered. It is important to first define what exactly is meant by a shock regime, and how it differs from other regimes we have discussed. In the shock regime loading rates are so extreme that structure behavior falls more under the umbrella of compaction/crushing, and can be more independent of the underlying structure than behavior at lower strain rates - aside from the influence from voids and impedance mismatch upon the propagation and reflections of the shock waves. A propagating shock is further followed by release, or rarefaction waves, which reduce the high pressure in the wake of the shock front. As defined by Forbes, the crucial differences between shocks in condensed matter and acoustic waves arises with the presence high pressure, mass particle speed, and internal energy changes in the case of a shock [110], all of which are lacking or greatly reduced

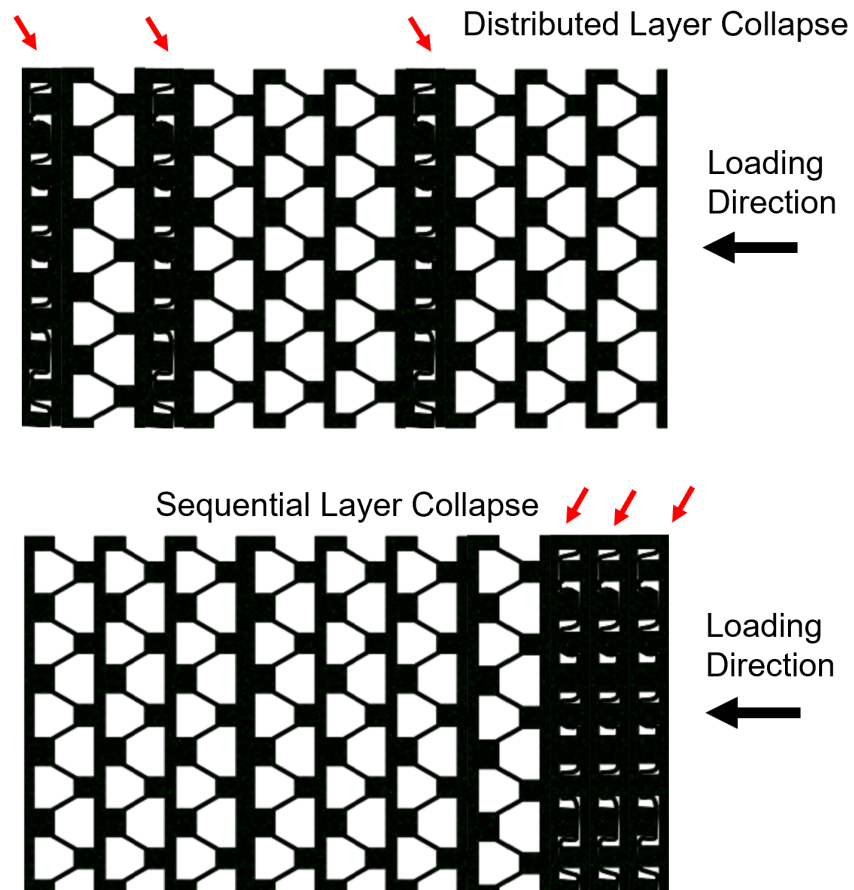


Figure 1.4. A visualization of random but uniform layer collapse of an architected material (top) vs. inertia-driven, sequential layer collapse (bottom). The red arrows highlight collapsed layers.

in acoustic waves. We note also that when the word ‘shock’ is used here, it refers to a regime that is qualitatively different from the lower strain rate, impact-induced successive collapse of layers in architected materials (noting that this phenomenon is sometimes also referred to as a type of shock in various literature). Here shock refers to what is sometimes called compaction shock within the context of layer collapse in architected materials [95, 111].

Due to the presence of a sharp discontinuity of pressure, stress, and strain in the material, the treatment of shock scenarios uses conservation equations to construct discontinuity, or jump, equations describing the behavior of the material in front of and behind the shock front. As outlined in Forbes [110], for a single 1D steady planar shock, the relevant equations can be derived by considering the conservation of mass, the change in internal energy, and Newton’s second law. The resulting conservation equations are

$$\frac{v}{v_0} = \frac{(U_s - u_p)}{U_s} \quad (1.4)$$

,

$$P = \rho_0 U_s u_p, \quad (1.5)$$

$$E - E_0 = \frac{P(v_0 - v)}{2}, \quad (1.6)$$

where U_s is the shock velocity, u_p is the particle velocity, E is the internal energy, P is the pressure, $v = \frac{1}{\rho}$ is the specific volume, and the subscript 0 refers to parameters in the un-shocked portion of the material. With these equations, it is possible to map between the un-shocked state and the ending, shocked state for a given material. This mapping draws out a curve in the $P - v$ or, equivalently, $P - u_p$ plane, referred to as the Hugoniot [110, 112, 113], an example of which is shown in Fig. 1.5. The linear compression path for each point along this curve, connecting the un-shocked state to the end state, is called the Rayleigh line. The building of a Hugoniot curve

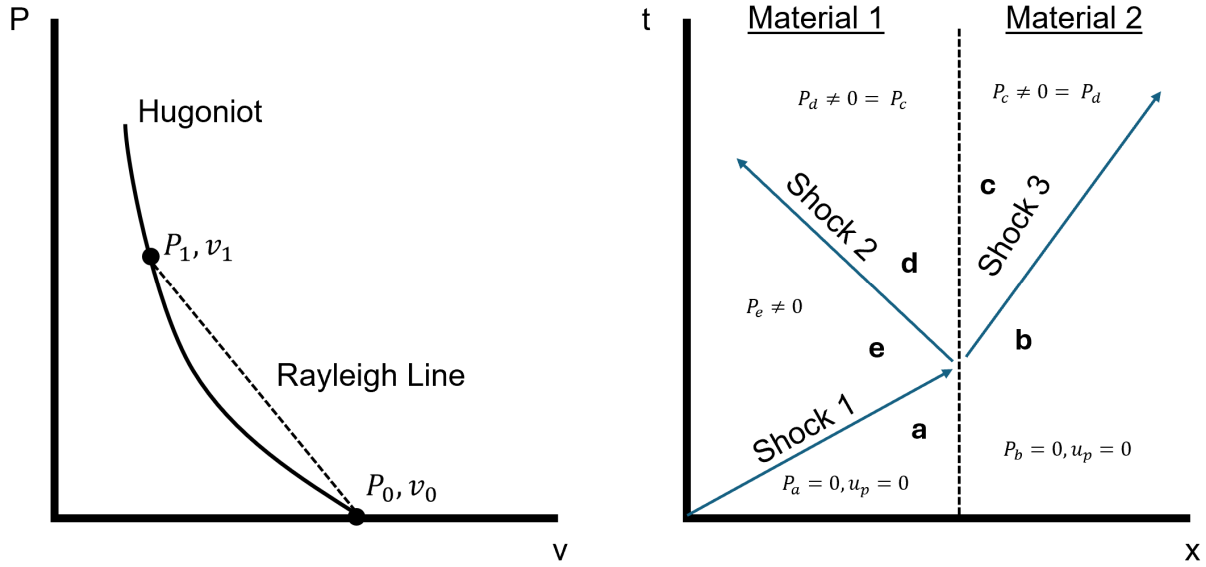


Figure 1.5. Left: An example Hugoniot and Rayleigh line of a shocked material. Right: An example x-t diagram showing the propagation and reflection of a shock wave from a material interface, used for impedance matching.

requires repeated shock experiments to obtain data for multiple points along the curve.

An important technique in tracking the propagation of shock waves and the properties associated with various pressure states is impedance matching [110]. Impedance can be defined as a measure of a material's ability to resist compression or generate pressure under loading, and shock impedance can be taken as the slope of the Rayleigh line connecting two states. When examining the propagation of a shock through space and time, the path of the shock and its reflection from boundaries can be visualized in an x-t diagram, as shown in Fig. 1.5. States at various portions of the x-t diagram can be determined by referring back to the Hugoniot curve of the materials involved and applying boundary conditions and the conservation equations (Equations 1.4-1.6). The value of the impedance determines the states upon reflection, highlighting how boundaries with an impedance mismatch in the path of a shock can be used to shape its propagation. This has been demonstrated by the use of structured voids in polymer structures [114] and the extensive use of foams [115–122] for shock attenuation.

There exist important failure modes which often occur in the shock regime. Of particular

interest to scenarios of impact mitigation is spall. This failure mode is the result of an impact event, in which compression waves reflect back from the free surface of the impactor and the impacted body as release waves. Where these reflected waves cross, a region of tension loading is created, which can result in the nucleation and growth of voids that tear the material apart [113, 123, 124].

Damage and failure due to spall phenomenon is highly dependent upon the material in question, depending upon material properties such as yield strength and ductility [125, 126], as well as the material microstructure such as loading direction with respect to sample orientation (both texture [127, 128] and crystallographic [129], grain boundaries [130], and grain size [125, 131, 132]. Experimental methods often involve shock loading samples via one of many available methods (gas gun driven flyer plates, laser induced shock, explosive detonation), and the measurement of the velocity history of the free (back) surface of the sample. From this information one can extract spall strength, the stress value at which spall initiates in a material, which can be approximated as

$$\sigma = \frac{1}{2}\rho_0 c_0 \delta u_{fs}, \quad (1.7)$$

in which σ is the spall strength, ρ_0 is initial (un-shocked) density, c_0 is the speed of sound, and δu_{fs} is the change measured in the free surface velocity associated with the arrival of the spall pulse [133, 134]. In addition to experiments measuring the spall strength, post-mortem examination of recovered samples has been used to provide information relating damage to the history of stress loading in the sample. Experiments with shock loaded and recovered samples have been used to deduce factors such as void nucleation rates, nucleation sites, growth rates, and coalescence, which have in turn been used to inform and tune analytical models [135]. Since spall onset and damage are highly dependent on the material in question, analytical models and simulations attempting to account for or predict damage often need to be tuned with experimental data for the material. This necessitates many experiments to properly parameterize models,

and makes accounting for the phenomenon in design approaches particularly difficult. Such phenomenon are therefore of interest to study further experimentally, in the hopes that better characterizing the behavior may lead to better models and enable their incorporation into design (and inverse design) attempts.

1.5 Dissertation Outline

The remainder of this work will delve into the challenges surrounding the high strain rate metamaterials. Chapter 2 contains the development of a topology optimization method for inversely designing polynomial type nonlinearities into a mesostructure. Chapter 3 outlines the coupling of this method with a reduced order discrete element model (DEM) for the purpose of incorporating waves and low strain rate dynamics. These chapters together provide a path for addressing the challenge of inversely designing for nonlinear wave tailoring. Chapter 4 then investigates the intermediate strain rate sensitivity of architected materials. This provides valuable insight into the dominant mechanisms in different strain rate regimes, such as when and how these mechanisms shift. Finally, chapter 5 experimentally investigates high strain rate, shock induced spall failure in metals, furthering efforts toward accurate modeling and characterization of behavior in the shock regime. This organization is outlined in Fig. 1.6

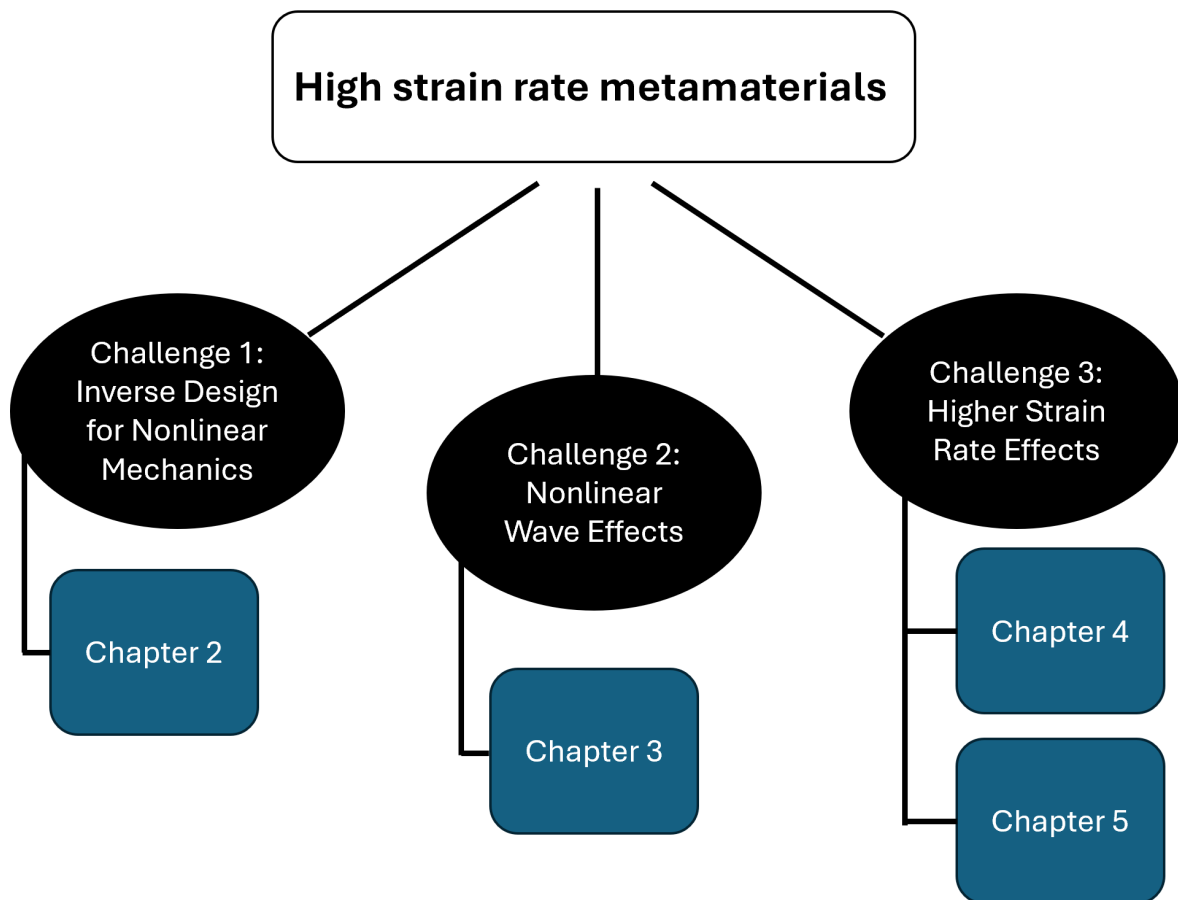


Figure 1.6. An outline of the organization of the dissertation.

Chapter 2

Tailoring high precision polynomial architected material constitutive responses via inverse design

The design of specified nonlinear mechanical responses into a structure or material is a highly sought after capability, which would have a significant impact in areas such as wave tailoring in metamaterials, impact mitigation, soft robotics, and biomedicine. Here, we present a topology optimization approach to design structures for desired polynomial nonlinear behavior, wherein we formulate the problem in such a way as to decouple the nonlinear response from the stiffness. We show results across qualitatively different polynomial behaviors while achieving a high degree of precision, creating a path toward analytically tractable nonlinear dynamical systems. The approach enables access to previously difficult to design for, or hitherto unachieved, nonlinear behavior via optimized structures, which can furthermore be incorporated as unit cells of designer materials with tailored nonlinear properties.

2.1 Introduction

Nonlinear behavior has been increasingly exploited to achieve useful mechanical effects. Recent work in acoustic, or “phononic”, metamaterials makes extensive use of unit-cell-scale structural features that exhibit nonlinear force-displacement laws to manipulate waves, inducing novel behavior such as dispersion tuning, harmonic generation, nonreciprocity, and solitary and rarefaction waves [76]. Explorations into impact and vibration mitigation, energy trapping, and energy harvesting have used nonlinearity to achieve drastic performance improvements [136–138]. Applications which involve large deformation regimes, such as soft robotics and bio-interface systems, rely upon the nonlinear response of their materials [58, 139, 140]. Further, in many mechanical signal processing and logic strategies, nonlinear responses are central to their functionality [141–144]. However, exploration of the role of different types of mechanical nonlinearities in such systems has been limited, due, in large part, to the lack of a general design approach for physically realizing desired nonlinear constitutive properties.

One approach for achieving tailorable nonlinear mechanical properties is to use geometric nonlinearity (*e.g.* large deformation or rotation, but small strain, effects). An important concept is that, within the context of metamaterial-like structured materials, the use of geometric nonlinearity allows the mesostructural geometric nonlinearity to transfer to an effective “material” nonlinearity (typically resulting in more nonlinear tailorability than, *e.g.*, chemical material synthesis methods). As such, the ability to tailor the nonlinear force-displacement response of structures can be considered applicable to both material and structural nonlinear response design problems.

Focusing here on future applications in nonlinear dynamics and waves in mechanical systems, we note that a rich body of research exists on systems that include polynomial nonlinear elastic elements [9, 76]. This is due, in part, to the ease with which polynomial nonlinearities can be treated analytically. Examples of canonical nonlinear dynamical systems include the Fermi-Pasta-Ulam-Tsingou (FPUT) system [145], which consists of polynomial intersite potentials,

and the ϕ^4 system, which is a subset of a nonlinear Klein-Gordon system, which consists of polynomial on-site potentials [146]. While discrete classes of polynomial nonlinearities have been studied in structured metamaterials, they are typically tuned around the local nonlinear response of known structures, and there has been little physically realizable exploration into the spaces in between these classes. Examples include contact nonlinearities [147], snap-through based structures [148], and tensegrity based structures [25]. This has relegated many potentially interesting nonlinear effects to analytical or computational treatment only.

Several inverse design approaches to alter a structure’s force-displacement curve have been previously explored. Topology optimization has been used to tailor a small number of force-displacement control points, often in the pursuit of designing snap-through structures [47, 48, 58, 59]. Improved energy absorbing materials have been designed by optimizing to increase the area associated with hysteretic paths traced by varied force-displacement curves [20, 66, 67]. A few works have explored the problem of optimizing a constitutive law over large strain ranges using trusses [34], splines [60, 61], and high fidelity topology optimization [22, 62, 149, 150]. More recently, investigations into the use of machine learning to seek specific force-displacement curves have been undertaken. However, such approaches sometimes result in imprecise matches with the desired responses, and often require the use of large training data sets [23, 24, 64, 65, 151, 152]. Importantly, none of the above-mentioned works pose the design problem in such a way as to be compatible with polynomial form nonlinearities – making the application to nonlinear dynamics, waves, and spring-mass models more difficult. In addition to qualitative differences observable in polynomial force-displacement relationships, such as symmetry around equilibrium or number of stationary points, there are also important, more subtle, dynamical differences that can emerge. For example, works such as Ref. [153] necessitate a precise balance between two nonlinear curves (in contrast to other, more forgiving, nonlinear objectives such as “plateau-like” behaviors sought after in low speed impact absorption). This is important when designing nonlinear springs because, at a superficial level, both springs would appear to have a qualitatively similar “stiffening” behavior in that region of the force-

displacement curve, but yield starkly different response in the frequency domain [154]. Matching force-displacement curves on a point-by-point basis may thus not be sufficiently precise to capture dynamic behaviors that depend upon what-appear-to-be minor differences between curves, but constitute stark differences in polynomial coefficients.

Here, we present a general approach for designing two-dimensional (2D), single material, nonlinear structures for a high precision one-dimensional (1D) nonlinear mechanical response. As schematically shown in Figure 2.1 A-C, we employ a level set topology optimization method, combined with mechanical intuition in the design of initial conditions, and target ratios of fitted polynomial coefficients as the objective function. The key aspect of our implementation is that the response is expressed as a ratio of polynomial terms, allowing easy access to the wealth of institutional knowledge of polynomial-form nonlinearities, as well as well established analytical and dynamical tools which are designed to handle nonlinearities of this form. In addition, considering the targeting of ratios, this approach allows us to decouple the optimization problem from the magnitude of structural stiffness within each design iteration, enabling the design to soften or stiffen as needed to achieve the desired degree of nonlinear behavior. Thereafter, the design can be scaled by adjusting the constituent material modulus, or size of the structure as is shown in Figure 2.1 C-E. This approach focuses the optimizer solely on the shape of the nonlinear response, circumventing the complexities of stiffness-nonlinearity dependencies. As such, it simplifies the inherently highly nonlinear design space to allow successful inverse design for targeted nonlinearities with precision. In other words, it is capable of exploring more design options and reliably finding solutions to a wider range of nonlinearities. Finally, the use of the level set method provides us with only the binary and smooth designs, enabling immediate manufacturing without post-processing, maintaining precision of the design (as opposed to density-based approaches, which often require post-processing and may lose some design precision in the process). The optimized nonlinear structures found herein can be incorporated into microstructures, lattices, or chains of springs and masses to form effective bulk material nonlinearities in pursuit of targeted designer materials. Geometric nonlinearity can be treated

as an effective material nonlinearity through consideration of a system of multiple unit cells, consisting of repeated optimized structures, as contributing to an effective, homogenized, higher scale bulk behavior (see Figure 2.1E for an example). We demonstrate the successful optimization of structures for multiple classes of nonlinearities achieved in the prior literature without employing the same microstructural mechanisms typically associated with said nonlinearities. In addition, we show a semi-continuous sweep across the linear plus cubic design structural response space, demonstrating the ability to fine tune structures reliably for highly specific forms of nonlinearity, rather than only broad classes.

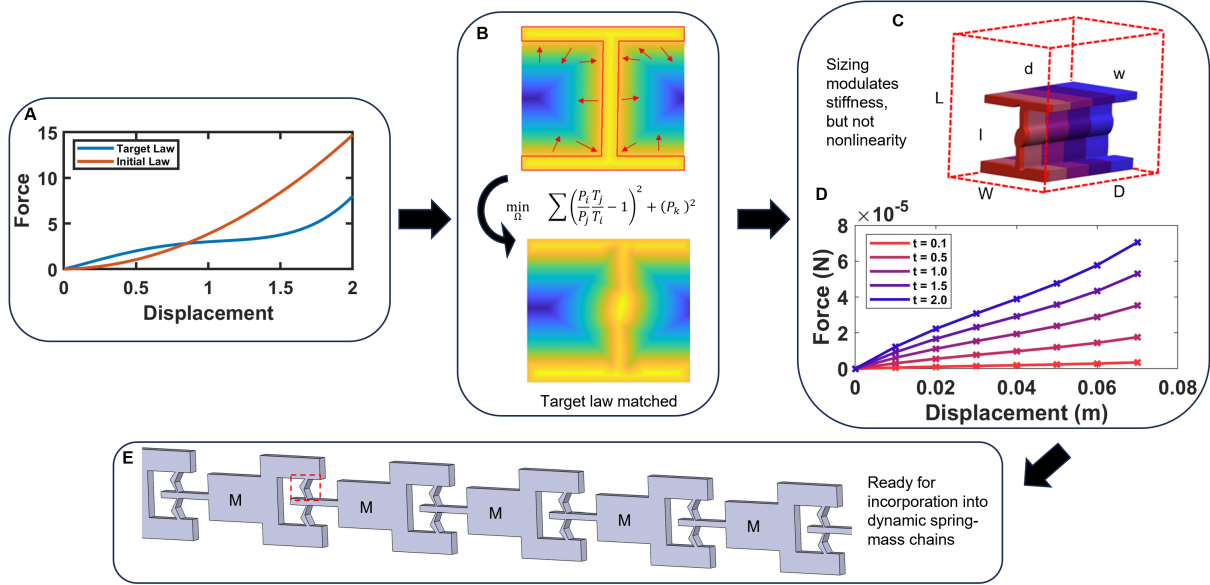


Figure 2.1. An overview of the proposed methodology used to design structures for targeted nonlinear mechanical behavior. A-B) A visualization of the level set approach for targeting coefficient ratios of a polynomial fitted to the force-displacement law shown in Panel A noting that the initial law shown is arbitrary, and depends upon the chosen initial condition, while the target law shown is the softening-to-stiffening target law displayed in Figure 2.3C). The solid red line in Panel B indicates the location of the zero level set, or the boundary of the structure, which is updated with each iteration as the design is changed. Blue and green indicate negative level set values (points outside of the structure), while yellow indicates positive level set values (points inside of the structure). Equation 2.1, the formulated objective, is shown in Panel B. C-D) A demonstration of how the stiffness of a structure (C) can be scaled by varying the out of plane thickness without affecting the shape of the nonlinearity (D), enabling designing for nonlinear behavior independent of stiffness, while still allowing for the modulation of global structural stiffness post design process. E) A visualization of how an optimized structure might be incorporated as a nonlinear spring in an example spring-mass chain (in which M refers to large masses, relative to the mass of the springs), forming an effective bulk nonlinear material. We note that this example is non-exhaustive, and that there are many ways in which such a nonlinear spring could be incorporated into a bulk nonlinear material.

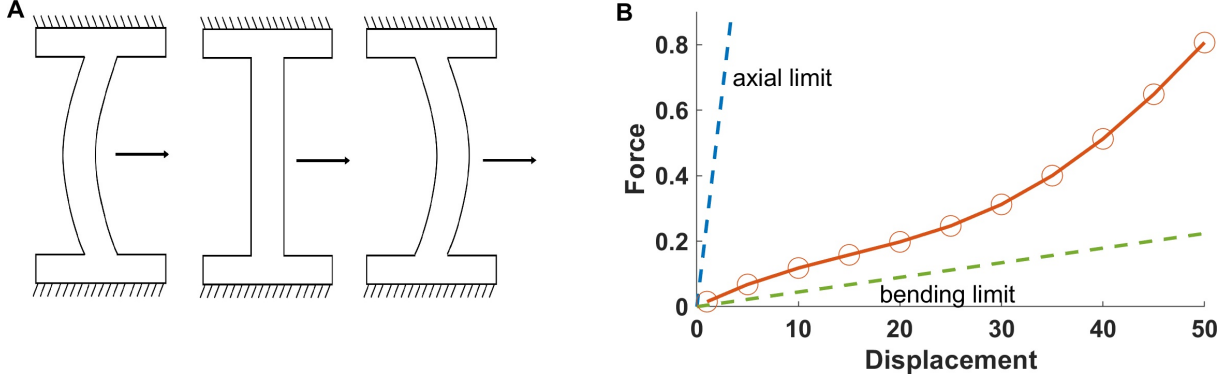


Figure 2.2. A demonstration of the mechanisms of geometric nonlinearity and their associated small deformation limits. A) A beam which uses geometric nonlinearity to achieve a softening to stiffening nonlinearity. B) The force-displacement curve of the beam in panel A (orange, circles), along with the limits calculated using the maximum and minimum stiffness from a full axial (top dashed line) and full bending (bottom dashed line) linear loading regime, respectively. These limits assume no negative stiffness in the structure.

2.2 Results

2.2.1 Heuristic Nonlinear Spring Design Method

As a first step to our general design methodology, we examine how to achieve broad classes of nonlinearity in a structure. Qualitatively, a softening nonlinearity can be achieved by transitioning a beam-like structure via large deformation and rotation from an axial-dominated loading regime to a bending dominated loading regime, while a stiffening nonlinearity can be achieved by reversing this transition (see, *e.g.*, Figure 2.2 A). By tailoring the shape of the structure, we can adjust both the amount of softening and stiffening and where these regimes exist in the deformation range. This can be done in either a single “spring” (in which, herein, we refer to a beam-like structure undergoing large deformation as our spring), or through a combination of multiple springs in series or in parallel forming an effective spring. We note that within the context of linearized stiffnesses, the stiffness of the overall structure will be dominated by the stiffness of the softer spring for springs in series, while the stiffer spring will dominate for springs in parallel. The resultant behavior can thus be tailored to produce the desired type of nonlinear behavior in the desired displacement or force region.

Parameters of importance can be identified by examining the case of a straight or curved beam being pulled through a fixed displacement range as shown in Figure 2.2 A. A spring of this general design could easily be incorporated into a spring-mass chain, with a mechanical frame present to enforce rigid boundary conditions, as displayed in Figure 2.1 E. Considering a system of this design, we take the beam highlighted in the dotted red box in Figure 2.1 E as our design domain. There exist inherent limits in how stiff or soft this structure can be made, and similarly, the magnitude of forces that can be reached in a given displacement range. Consider first the blue dashed upper line in Figure 2.2 B, which corresponds to the limit EAL^{-1} and describes linear stiffness corresponding to the axial deformation of a long, thin elastic beam, where E , A , and L are the beam's elastic modulus, cross sectional area, and length, respectively. This limit can be interpreted to define the approximate maximum force that could be achieved at a given deformation δ , by pulling a beam that extends normally from a fixed boundary, in an axial fashion. Such a regime could be imagined to be achieved when the beam in Figure 2.2 A is pulled far to the right ($\delta \gg L$). This further serves as a small ($\delta \ll t$, where t is the beam width) and very large deformation ($\delta \gg L$) limit on the structural stiffness, with implications for the effect of volume ratio in an inverse design method on achievable stiffnesses. An exception to these limits, as concerns local stiffness at intermediate displacements is the case of snap through and snap back (or snap down), where infinitely positive, infinitely negative, and zero local stiffnesses can be achieved [155]. For instance, considering a structure that exhibits a single snap through or snap back feature, we could expect the following. For both a snap-through and snap-back structure, there is guaranteed to be two points of zero stiffness. For a snap-through structure, there is also guaranteed to be a point of finite negative stiffness which approaches a vertical slope in the limit of snap-back behavior. This vertical slope could be considered as an infinitely positive or negative stiffness. For a snap back structure, there is similarly guaranteed to be two points of vertical slope. Similarly to the blue dashed line forming the upper limit, we can define an approximate lower bound, denoted by the green dashed line in Figure 2.2 A for stiffness in small deformation ($\delta \ll t$) regimes, which corresponds to the EIL^{-3} bending stiffness of a long

thin beam, with I being the second moment of area. The exception to this bound would be to include contact effects, or to include a pre-load on a structure exhibiting negative stiffness onset. Without considering contact and pre-loads, this has important implications for the dependence of the small deformation stiffness that can be achieved on the structure's minimum feature size.

Within the aforementioned bounds, we suggest that a wide range of qualitatively different nonlinear force-displacement paths, which can be fit by a polynomial (as a function of displacement/strain), should be achievable through this exploitation of geometry, even those which elsewhere in literature have been achieved through other mechanisms, mechanical or otherwise (*e.g.*, magnetism, etc.). Further, while these qualitative design guidelines are helpful, we look herein to topology optimization techniques to refine the design process for more exact targeted nonlinear behaviors.

2.2.2 Optimization Method

A 2D plane stress, geometrically nonlinear (large deformation), displacement controlled, level set optimization was implemented, following the method described in [38, 156]. For simplicity, we restricted this work to a tension regime. A Kirchhoff material model was implemented, allowing for geometric nonlinearity and large strains while maintaining a linear elastic material model. We choose a level set optimization method because of its compatibility with our pursuit of simply manufacturable, binary (material and no material) geometries. The inherently binary representation of the level-set approach leads to less required post-processing, and therefore easier manufacturing, of identified designs.

Within the context of the stiffness bounds described as part of Figure 2.2, we highlight that there exists an inherent coupling between the degree of nonlinearity and the stiffness of a structure (excepting phenomena related to snap through and snap back). We define degree of nonlinearity as the relative magnitude of nonlinear terms in the force-displacement relationship with respect to the linear term at a given displacement. To elucidate the coupling between nonlinearity and stiffness, we consider the transition between axial and bending deformation of

a long thin beam. Taking a ratio of those two characteristic stiffnesses (axial by bending) for a beam of rectangular cross section, we obtain a ratio of $(Lt^{-1})^2$, demonstrating that thinner structures are capable of greater change in stiffness (*i.e.*, nonlinearity) over a fixed displacement range. However, thinning a structure makes it softer, resulting in a uniformly lower magnitude force displacement curve. As mentioned above, many previous attempts at this problem have employed an objective function which attempts to directly target a force-displacement curve. This severely limits the design space, excluding multiple, and sometimes all, viable solutions. In that case, a better goal, in pursuit of a specific nonlinear behavior, is to search for geometries which will enable the desired strength and shape of nonlinearity, regardless of the stiffness of the structure. We address this by defining the objective function in terms of a polynomial that is fitted to the force-displacement curve, wherein the objective is set to match a desired ratio between polynomial coefficients. This objective is written as

$$\min \sum \left(\frac{P_i}{P_j} \frac{T_j}{T_i} - 1 \right)^2 + (P_k)^2, \quad (2.1)$$

where P_i and P_j represent the current design polynomial coefficients being optimized for a desired ratio, T_i and T_j represent the target ratio, and P_k is a current design polynomial being driven to zero. A target linear plus cubic polynomial constitutive law could thus be written as $F = T_j x + 0x^2 + T_i x^3$, while the current design's constitutive law would be written $F = P_j x + P_k x^2 + P_i x^3$, in which the ratio of the i and j terms would be optimized to match the target ratio, while the k term would be driven to zero. For targets which have multiple desired ratios, multiple j terms can be used. We note that, by optimizing for polynomial coefficient matching, a limitation is introduced, which restricts targeted nonlinearities to those which can be well-fit by a polynomial (this excludes behavior such as snap-back, for example, when using a polynomial that is a function of displacement). However, a wide variety of nonlinear curves can be well described by a polynomial fit, particularly as the order of the polynomial is increased, resulting in an extensive space of potential nonlinear targets to be explored.

Sensitivities for this objective function can be written as a combination of sensitivities for compliance and sensitivities related to the fitting of the polynomial. We calculate self-adjoint, nonlinear, displacement control compliance sensitivities, $\partial C_j / \partial \Omega$, as calculated in [156], where C is the compliance and Ω is the domain. Calculating our polynomial fit through use of the equation $P = V^{-1}C$, where V^{-1} is the inverse of the Vandermonde matrix, the sensitivity for each polynomial term is written as:

$$\frac{\partial P_i}{\partial \Omega} = \sum_{j=1}^m \frac{\partial P_i}{\partial C_j} \frac{\partial C_j}{\partial \Omega} = \sum_{j=1}^m V^{-1}(i, j) \frac{\partial C_j}{\partial \Omega}, \quad (2.2)$$

where i refers to the degree of polynomial, j refers to the displacement step, and m is the total number of displacement points under consideration. In addition, we employ a smoothing algorithm in the mapping of the sensitivities to the level set boundary nodes [157], which discourages very small, discontinuous notches and protrusions in the resulting design.

Despite the ability to identify gradients in the design space, we note that this particular inverse design problem is highly non-unique and non-convex. Hence, optimization can get stuck in local minima which may not be sufficiently close to the objective nonlinearity. In order to improve the quality of a solution, we use mechanical intuition to choose an initial condition that is qualitatively “nearby” the desired type of nonlinearity, through the heuristic spring design process described above. This narrows down the number of possible solutions the optimizer can reach, and reduces the chances of becoming trapped in an undesirable local minimum. A brief exploration of the effect initial condition choice can have on the ability to find a satisfactory local optimum is included in the SI. This approach, presented herein, requires some mechanical insight and designer input in choosing an initial condition. Similar approaches have been employed in other works, which have relied upon the input of reduced order training datasets [23] and the use of multiple initial condition guesses [22] to achieve the target constitutive behavior.

2.2.3 Examples

To demonstrate the capability of the design method and optimization process, we optimize several spring structures to target specific nonlinear constitutive laws from several classes of nonlinear behavior, *i.e.* softening, stiffening, softening to stiffening, and stiffening to softening. By optimizing a structure for each class of nonlinearity, we demonstrate the capability of the approach to span the nonlinear design space and target any type of nonlinearity that falls within the range of these classes. These results are depicted in Figure 2.3, in which the force-displacement equations with the following polynomial coefficients are targeted: Softening, $F = x - 40.0x^3$; stiffening, $F = x + 163.3x^3$; softening to stiffening, $F = 1.40x - 17.332x^2 + 166.875x^3$; and stiffening to softening, $F = 0.599978x + 17.332x^2 - 166.875x^3$. The displacement range was chosen arbitrarily, as were the coefficient weights, though in the latter two cases, the target polynomial coefficients were chosen to achieve symmetric stiffness switching springs, as outlined in [153]. Nearly all targeted nonlinearities were matched to within less than 1% of the desired coefficients (with the sole exception being the softening-to-stiffening case, discussed below). In the optimizations shown in Figure 2.3, the initial conditions were selected to be in the same class of nonlinearity as the desired target (for example, an initial condition which displayed a general stiffening nonlinearity was selected for the stiffening-type nonlinearities), with coarse adjustments being required to tune the initial polynomial coefficient signs. The initial conditions and polynomial fit details for each optimization case can be found in the SI. We suggest that all of the optimized designs can be considered “non-intuitive”, in that they would be difficult or impossible to design by hand to the desired degree of precision using human intuition alone. We draw particular attention to the two stiffness switching optimized designs shown in Figure 2.3 C and D, as these targeted constitutive laws were more complex in nature, requiring the optimizer to capture a qualitative shift in behavior and to perform optimization for two polynomial ratios simultaneously. The stiffening-to-softening spring design in Figure 2.3 D, in particular, is of note in that it can be considered to be the combination of two springs (beams) in series (one

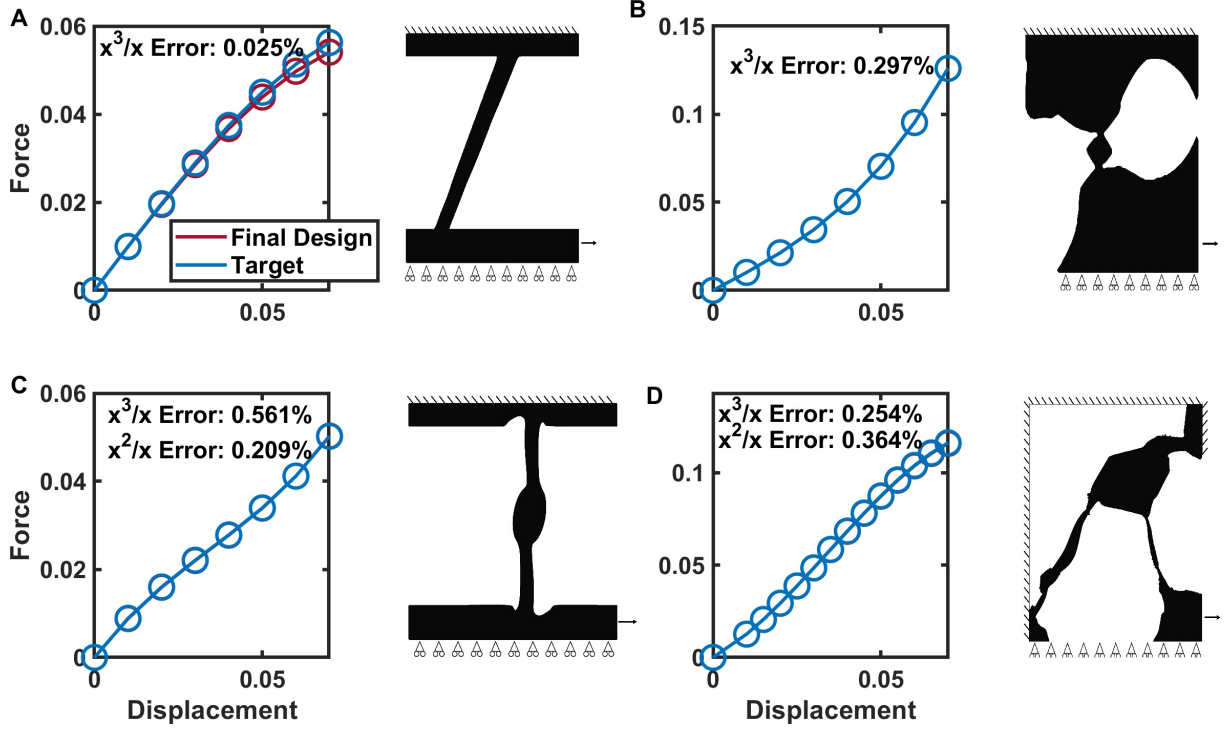


Figure 2.3. Optimized structures for four different classes of nonlinearity, including softening (A), stiffening (B), softening to stiffening (C), and stiffening to softening (D). The red curves represent the normalized polynomial law achieved by the design, while the blue represent the normalized target polynomial.

stiffening spring and one softening spring) in order to achieve the desired behavior. These two springs are highly coupled, with the nonlinear behavior of each affecting not only the overall behavior of the structure, but also the boundary conditions and applied displacement of the other spring, creating a highly complex and nonlinear design scenario. We note also that designs such as those in Figure 2.3D, with very thin and hinge-like components, may encounter difficulties with solver convergence due to the finite element mesh excessively distorting (see SI).

The optimization results demonstrate that the method is capable of designing a variety of nonlinear springs. The high degree of precision in matching a target behavior also makes it possible to target nonlinearities which vary from one another only slightly, sweeping through the design space for the desired nonlinear behavior. To demonstrate this capability, we chose a target which consisted of a linear plus cubic stiffening type nonlinearity ($F = x + Ax^3$), and varied the

target coefficient weights (A is varied). This type of sweep is fairly straightforward to perform once the first design has been optimized, as the optimum from one design can be used as the initial condition for the next step, in many cases (but not all) eliminating the need to design the initial conditions. The results are shown in Figure 2.4. We first draw attention to the distinct shift in design between ratios 40 and 80. This transition represents a local minimum which led to a relatively poor optimization of the ratio 40 target, and prevented an acceptable optimization of the ratio 20 design from an initial condition drawn from this poor ratio 40 optimization. Intuitively, this makes sense, as the hinge-like structure present in the more nonlinear designs is qualitatively different from the type of structure which might be expected to exhibit more linear behavior. Selecting a new starting design, which in this case consisted of straight edges and a thicker beam to promote a weaker nonlinearity, provided a successful workaround which avoided the local minimum and found a satisfactory design for the ratio 20 target, as well as an improved optimal design for the ratio 40 target. This difficulty highlights the challenges of the highly nonlinear design space, and the ease with which such local minima can be circumvented with educated initial design. We also note that the coupling of stiffness and nonlinearity is clearly visible in the optimized curves of the sweep designs (considering ratios 40-163 to be grouped together, and ratios 10-20 to be grouped together) in Figure 2.4B, in which the more linear designs display stiffer overall behavior, while the more nonlinear designs are softer. This change in nonlinearity (and stiffness) is achieved by increasing or decreasing the thickness. We highlight this in the zoomed-in images of the ratio 40-163 optimized structures in Figure 2.4, noting that the ratio 163 design is the optimized stiffening design from Figure 2.3, and that each subsequent ratio uses the optimum from the previous ratio as the initial condition.

With respect to the coupling between stiffness and nonlinearity, while, as in Figure 2.1, it is simple to normalize or scale the linear stiffness (or resulting force magnitude) computationally, we also note that there are several mechanisms to achieve this in practice. Perhaps the most straightforward manner to scale the resulting stiffness or effective modulus would be to adjust the elastic modulus of the constituent material forming the design. However, in practice, materials

occupy discrete moduli ranges and come with other practical limitations such as small elastic ranges. As an alternative approach, consider first the structural stiffness of the design. To keep the same degree of nonlinearity, while increasing the magnitude of the force (thus compensating for the normalized stiffness), one could change the depth of the 2D geometry, as shown by the varied colors in Figure 2.1C and the resulting force-displacement curves in Figure 2.1D. One could also scale the area of the 2D geometry, thus increasing the force, however, the applied displacement must also be proportionally scaled to achieve the same degree of nonlinearity. We next consider scaling the response from the perspective of an effective stress-strain response. Consider the 2D design with a nonlinear stiffness $k(\delta)$ is assigned some depth d , length l , and width w , as shown in Figure 2.1C. This structure is then repeated within a larger unit-cell domain of depth D , length L , and width W , wherein the designed region is attached to a rigid frame as shown in Figure 2.1E. The resulting stress strain relationship would thus be $\sigma = \epsilon kL(DW)^{-1}$, such that the size of the unit cell becomes essentially a single scaling factor equivalent to scaling the modulus of the constituent material. There is a key difference from scaling the constituent modulus, however, where the lengths defining the design domain cannot exceed that of the larger, unit cell domain.

Furthermore, we include several additional examples of optimizations in order to demonstrate the range and versatility of the method. While the examples above highlight distinct nonlinear behaviors, several of the targeted curves are weakly nonlinear. To demonstrate that the method is not constrained to weak nonlinearities, Figure 2.5A highlights a targeted stiffening curve displaying a greater degree of nonlinearity (and a purely quadratic constitutive law). The target in this case is $F = x + 200.0x^2 + 0x^3$. We note that, when the maximum displacement of 0.07 is substituted into x in this target, the ratio of the quadratic term to the linear term becomes 14, demonstrating an order of magnitude difference between linear and nonlinear terms. In Figure 2.5C, a constitutive law containing a fourth order term is targeted in order to show that the above cubic examples are an arbitrary choice of nonlinearity, and there is nothing constraining the method to third order terms. In addition to targeting the distinct nonlinear behaviors

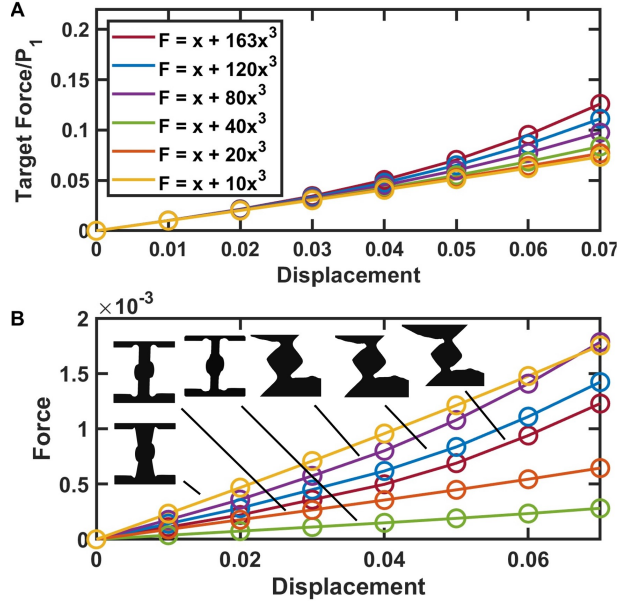


Figure 2.4. Optimized springs resulting from a sweep of the nonlinear term in the force displacement equation $F = x + ax^3$, in which a is varied from 10 to 163. A) Normalized results, wherein the linear stiffness has been divided out such that all curves have a uniform linear stiffness. B) Non-normalized results, in which curves have been left with the varied linear stiffness directly from the optimization results, highlighting the stiffness variation that is exploited in the optimization process to achieve varying degrees of nonlinearity. The non-normalized force-displacement equations are as follows, in order of descending nonlinearity: $F = 0.0104 - 0.0004x^2 + 1.7002x^3$, $F = 0.0136x - 0.0026x^2 + 1.6352x^3$, $F = 0.0171x + 0.0038x^2 + 1.3460x^3$, $F = 0.00377x - 0.0072x^2 + 0.1498x^3$, $F = 0.0089x - 0.0087x^2 + 0.1784x^3$, $F = 0.0232x + 0.0097x^2 + 0.232x^3$. The snapshots of the three optimized structures on the right (target ratios of 80 to 163) are zoomed in on the high sensitivity regions. The full structures can be found in the SI.

outlined above, we desire the capability of targeting nonlinearities which lie in the negative stiffness, as well as fully bistable regime (a capability which is highly useful in pursuing superior impact-resistant structures.) [136] One benefit of our displacement-controlled approach is the capability to solve problems which exhibit negative stiffness and snap-through type behavior with a Newton-Raphson solver. In Figure 5B below we show optimizations which target a fully bistable force-displacement curve. Results of an optimized negative stiffness (but not fully bistable) structure are shown in Figure 5D, for a targeted nonlinear law of $F = x - 10.0x^2 + 30.004x^3$. For both of these cases, we optimize over a greater displacement range in order to more easily realize the more nonlinear negative stiffness behavior without resorting to a significantly increased mesh density (as would be required for a thinner structure). As above, the displacement range and targeted nonlinearity are otherwise arbitrary. This optimization requires the simultaneous optimization of two ratios. For the initial optimization run, both ratios were matched to within 1% (0.638% for the cubic and 0.636% for the quadratic). However, in this case, the negative stiffness portion of the curve is heavily dependent upon only one of these two ratios (the quadratic, which is responsible for the transition to negative stiffness due to the negative sign associated with the term), and the behavior in the negative stiffness region is accordingly much more sensitive to this ratio. We therefore add a weight (a 10x multiplier) to the quadratic ratio for this optimization, prioritizing this term over the cubic term. This result (shown in Figure 2.5D) achieved a lower match to the cubic term (1.712%), but a much closer match to the prioritized quadratic term (0.180%), resulting in a closer normalized match of the negative stiffness portion of the curve.

2.2.4 Experimental Verification

In order to confirm the accuracy of the method and the validity of the optimized springs, several of the springs shown herein were chosen for manufacturing and experimental verification of the nonlinear force-displacement curves. Polycarbonate was initially chosen to fabricate the springs from, due to its relatively linear behavior at lower strains and high strain-to-break value. However, preliminary tests indicated that for thicker structures, plasticity onset (which is not

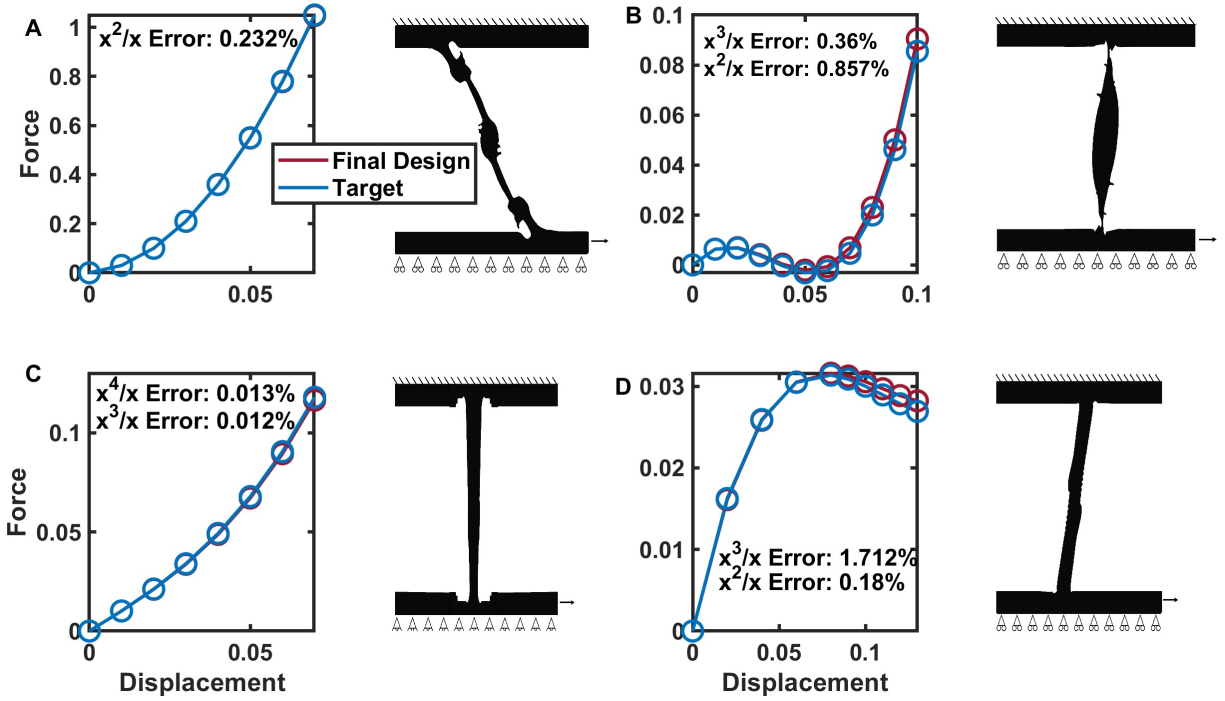


Figure 2.5. Additional optimization examples, highlighting the versatility of target-able curves. A) A purely quadratic, highly nonlinear stiffening optimization. B) A bistable optimization. C) A fourth order optimization. D) A negative stiffness (but not fully bistable) optimization.

accounted for in the optimization's Kirchhoff material model) would introduce unaccounted nonlinear behaviors. The thinnest structures, the bistable spring from Figure 2.5B and the stiffening-to-softening spring from Figure 2.3D, were therefore manufactured and tested in polycarbonate, with the results shown in Figure 2.6A and E indicating close agreement between optimization outputs and experiments. It is of note that such experimental validation proved to be incredibly sensitive to misalignment issues (such as any out of plane offset or the direction of displacement application not being precisely horizontal) and quality of the boundary condition approximation. Regarding the latter, the imposition of the y-direction being fixed on the top and bottom edges via the frame containing the optimized structure, in particular, was found to be very important, due to a great deal of the nonlinearity stemming from the structure pressing against these surfaces during deformation. Indeed, insufficient stiffness of the frame, or lateral forces applied to it, were observed to modify the resulting nonlinear force-displacement response of the designed structure. This was particularly true for the case of the bistable spring. Careful

construction of the system was thus required in order to achieve good experimental match, which may require additional attention when considering real-world applications. We also note that, due to the FE simulations being run on a 1x1 m domain, often with a modulus of $E = 1$ Pa, simulation results required scaling to match up to experimental results. This is to be expected, and highlights the ability to manipulate the scale of the structure in order to achieve desired force ranges. Simulation results were scaled along the x-axis by the size of the unit cell (*i.e.*, experimental unit cell length/simulation unit cell length), and along the y-axis by the modulus of the constituent material used in the experiment (found via scaling max and min values of nonlinear curves, as described in the SI), the edge length of the unit cell, the depth, and a factor of two to account for two springs being present in the experiment (*i.e.* experimental unit cell length/simulation unit cell length), and along the y-axis by the modulus of the constituent material used in the experiment (found via scaling max and min values of nonlinear curves, as described in the SI), the edge length of the unit cell, the depth, and a factor of two to account for two springs being present in the experiment (*i.e.* $(E_{Exp}/E_{Sim}) * (L_{Exp}/L_{Sim}) * (D_{Exp}/D_{Sim}) * 2$, in which E refers to Young's Modulus, L refers to the edge length of the unit cell, D refers to the depth of the unit cell, subscript Exp refers to the value in the experiment, and subscript Sim refers to the value used in the optimization).

As the ability to test any optimized structure was desired, an updated material model was introduced to the modeling for optimization, which would allow for the use of fabrication materials that exhibit a larger elastic range. A Neo-Hookean (hyperelastic) material model was introduced, with a plane strain formulation. The softening to stiffening spring shown in Figure 2.3C, which exhibited a relatively thicker design, was re-run with the updated material model, beginning from the optimal configuration identified with the Kirchhoff material model. Small adjustments were made to the design by the optimizer to account for the new material model. This updated structure was then fabricated out of silicone (see SI for material and fabrication details) and tested. The results, shown in Figure 2.6B, demonstrate that the updated material model has similar levels of agreement to the original Kirchhoff material model, and allows for

the fabrication and testing of thicker structures while avoiding the onset of plasticity. We note that analogous scaling was performed to map between simulation and experimental results, as described above in the elastic case. Further information on experimental validation is included in the SI.

2.3 Conclusion

The optimization design methodology developed herein targets polynomial material or structural constitutive response coefficient ratios, decoupling the desired nonlinear behavior from the inherent stiffness in its description. Through this, we bypass the limitations associated with stiffness-nonlinearity coupling. We have demonstrated the capability to design nonlinear springs with both breadth and precision. With desired high-precision nonlinear behavior having importance in areas ranging from impact mitigation to wave tailoring metamaterials, compliant mechanisms, mechanical logic and signal processing, soft robotics, and biomedicine (particularly settings involving biological-synthetic interfaces), we envision this approach enabling the development of new designer materials within these areas.

Future near-term potential applications of this method may include the experimental implementation of several 1D chains, as proposed in Figure 2.1E (*e.g.* [153, 158] and impact-mitigating mechanical metamaterials. While 1D chains are an area of rich physics in which to validate the implementation of the method described herein, the extension to 2D, and furthermore three-dimensional (3D), are expected to present a host of new challenges. A system in which each unit cell interacts nonlinearly with the one next to it, and in which the nonlinear response is expected to be characterized by multiple degrees of freedom, introduces an increased degree of complexity which bears future examination. Such advancements will help enable tailoring of 2D or 3D bulk materials for loading in multiple directions.

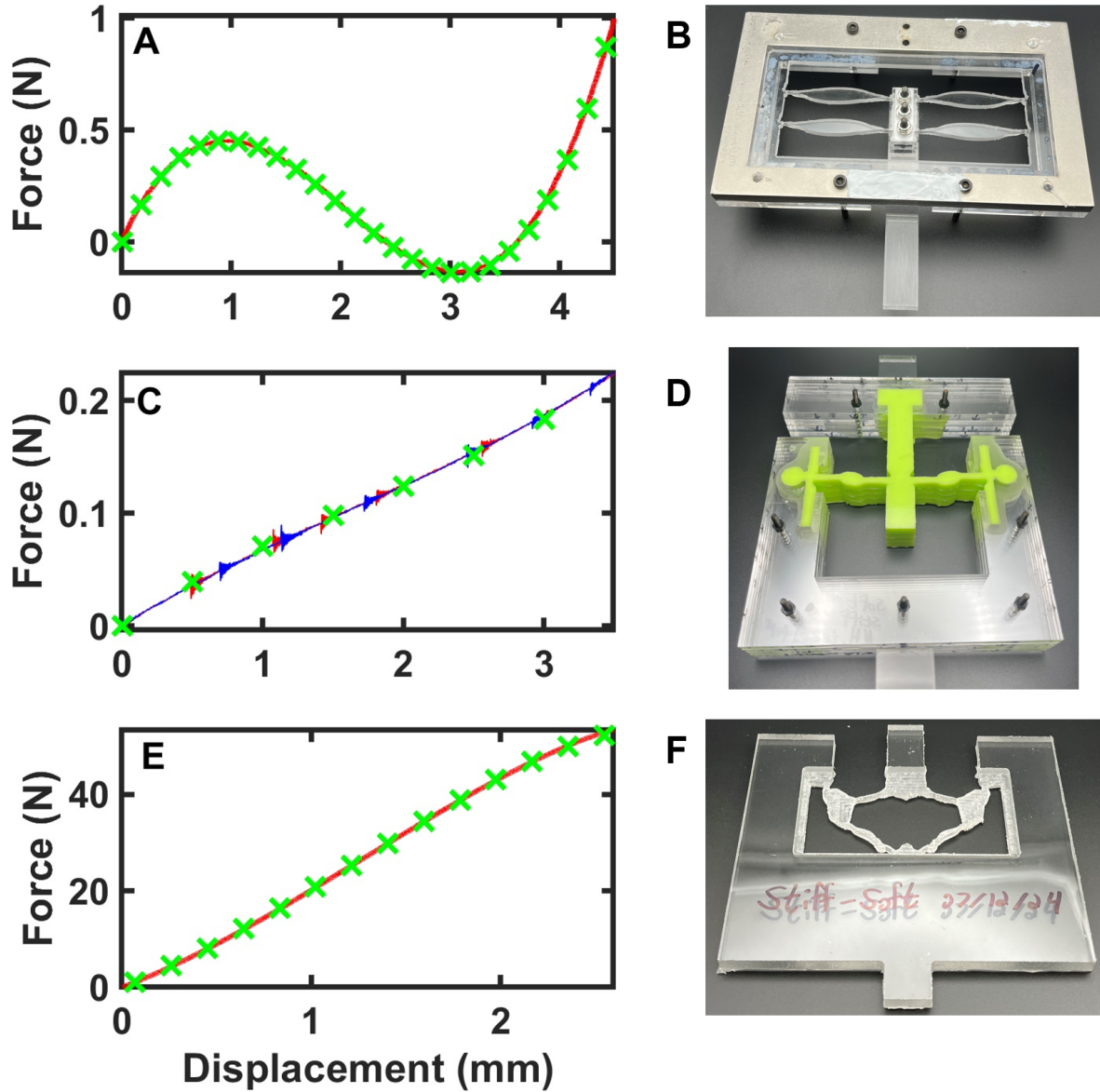


Figure 2.6. Experimental validation of optimized spring force-displacement curves, in which red and blue solid lines indicate experimental data, and green x markers are overlaid simulated force-displacement curves. Shown are A-B) the bistable optimized spring shown in Figure 2.5B (fabricated from polycarbonate, in which the frame has dimensions from top edge to bottom edge of 92.7 mm), C-D) the softening-to-stiffening spring shown in Figure 2.3C (fabricated from silicone, in which the frame has dimensions from top edge to bottom edge of 140 mm), and D-E) the stiffening-to-softening spring shown in Figure 2.3D (fabricated from polycarbonate, in which the frame has dimensions from top edge to bottom edge of 101.7 mm).

2.4 Supplemental Information

2.4.1 Polynomial fitness values

We include here details about the polynomial fitting process, the quality of the final polynomial fits, and the initial conditions.

As described in the main text, the polynomial fitting algorithm is performed using the Vandermonde matrix, using the equation $P = V^{-1}y$. Here, y is taken to be compliance C , where $C = xf$, where x is the applied displacement, and f is the reaction force at the nodes which are under a nonzero applied displacement boundary condition. The polynomial fit is performed to compliance, rather than directly to the force, for ease of sensitivity calculations. This results in an extra x term being included in the fit, which shifts the polynomial fit up one order. This is addressed by dividing out the extra x term, and shifting the polynomial order down one. For example, a fit to compliance of $C = ax + bx^2 + cx^3 + dx^4$ is equivalent to a fit to force of $F = bx + cx^2 + dx^3$.

Every polynomial fit naturally has some small fitting error associated with it. For completeness, we include the R^2 values in Table 2.1 below. These values highlight the high degree of accuracy in the polynomial fits performed in the optimization process.

In addition, we include in Table 2.1 an alternative error measurement in the form of percent difference values between optimized and target normalized force-displacement curves. While this value in most cases highlights the excellent agreement between optimized and target curves, we note that there are several cubic stiffening sweep targets with integrated error across the curve on the order of 10%. This error is driven by a somewhat high, nonzero quadratic term, which was desired to be driven to zero. We note that in the cubic stiffening cases, the nonlinear ratio of the cubic to linear terms was prioritized over the quadratic term. If, however, a more precise curve match is desired in these cases, a weighting term can be added to the quadratic term, as described in the main text, to place a higher priority upon this objective, and reduce the error associated with this term.

Table 2.1. Polynomial Fit Details

Target Polynomial (Normalized)	Optimal Fitted Polynomial (Normalized)	R^2	Ratio Error (x^2/x)	Ratio Error (x^2/x)	Integrated Curve Error
$x + 163.3x^3$	$x - 0.04x^2 + 163.78x^3$	0.999	0.297 %	NA	0.0508 %
$x - 40.0x^3$	$x - 0.45x^2 - 40.01x^3$	0.999	0.025 %	NA	2.341%
$x + 28.887x^2 - 278.135x^3$	$x + 28.782x^2 - 277.429x^3$	0.999	0.141 %	0.254 %	0.364%
$x - 12.380x^2 + 119.196x^3$	$x - 12.405x^2 + 119.865x^3$	0.999	0.561 %	0.209 %	0.191 %
$x - 10.0x^2 + 30.004x^3$	$x - 9.936x^2 + 30.195x^3$	0.999	0.638 %	0.636 %	1.02 %
$x + 120x^3$	$x - 0.188x^2 + 120.180x^3$	0.999	0.15 %	NA	0.646 %
$x + 80x^3$	$x + 0.225x^2 + 78.598x^3$	0.999	1.753 %	NA	0.590 %
$x + 40x^3$	$x - 1.91x^2 + 39.71x^3$	0.999	0.736%	NA	8.19%
$x + 20x^3$	$x - 0.977x^2 + 20.045x^3$	0.999	0.225 %	NA	4.38 %
$x - 41.064x^2 + 396.11x^3$	$x - 40.712x^2 + 397.535x^3$	0.998	0.36 %	0.857%	6.926%
$x + 200x^2 + 0x^3$	$x + 199.536x^2 - 0.272x^3$	0.999	NA	0.232 %	0.216%
$x + 0x^2 + 150.0x^3 - 150.0x^4$	$x - 0.294x^2 + 150.018x^3 - 150.020x^4$	0.999	0.012%	NA	1.02%

2.4.2 Initial conditions

The initial conditions from the optimizations are included in Figs. 2.8, 2.9, and 2.10 below. We highlight that these are simple, intuitive designs which required minimal designer input (with the possible exception of the stiffening-to-softening condition, which required the designer to choose springs in series as the initial design). Most cases were run with initial conditions that consisted of simple straight beams. In the stiffening and stiffening to softening cases, however, conditions which consisted of circular holes were explored to investigate the effect of more random starting points. It was found that the optimization still performed well and converged to an acceptable solution, and that the hole-based boundaries had little impact aside from producing more irregular optimum designs (e.g., containing protrusions and excess material which had little impact on the nonlinear behavior). This dependence of the final design upon the initial condition is expected, due to the high nonlinearity and non-uniqueness of the design space. A brief exploration of initial condition dependence was conducted, in which a simple cubic stiffening optimization was attempted with a coarser mesh. The same problem was attempted with several different initial structures, the results of which are shown in Figure 2.7. The results highlight the extremely nonconvex nature of the design space, as well as the dependence of not just the final structure, but the best achievable performance (the quality of the best achievable local minima), upon the choice of initial structure. For this simple stiffening nonlinearity, the initial condition shown in Figure 2.7A is able to easily manipulate the polynomial coefficients to

find a decent local optimum. This is not surprising, given that this initial condition begins in a configuration from which stiffening type behavior can be easily achieved, and thus is relatively close to a region with a desirable local optimum. The initial condition shown in Figure 2.7B consists of an array of regularly spaced holes, and is likewise able to find a decent local optimum, although not as close of a match as that from Figure 2.7A and more complex in manufacturing. It can be seen in Figure 2.7C, however, that an initial condition which begins far away from the desired stiffening behavior is unable to find a local optimum 'close enough' to the desired coefficients. In this case, the initial condition is a strongly softening type nonlinearity, and qualitatively different to the point that we expect that there is not a local optimum nearby. Finding a good optimum from this configuration would require navigating the highly nonlinear design space without getting trapped in a non-ideal local minimum with which a gradient-based optimization method struggles. Options for dealing with this include introducing some method of kicking the design out of the local minimum in a stochastic way, running many initial conditions and choosing the one which finds the best local optimum, or informing initial condition choice with mechanical insight to increase the chances of beginning near a good local optimum (whether this be insight from a reduced order model, or input from the designer). We choose the last option, but note that other approaches are also viable.

We note that in some cases optimizations were first performed with a coarser mesh, with the design being refined by a subsequent finer meshed optimization. This is sometimes necessary to achieve accurate results when the optimization produces thin beams represented by only a few elements across the width, reducing accuracy of the FEM solve. All final optimized results were imported into COMSOL Multiphysics, and a finite element analysis was run with a body-fitted, triangular mesh, in order to verify the optimization results. The same material model and boundary conditions were used in Comsol as described in the main text. The meshing details can be found in Table 2.2. It should be noted that the optimization mesh includes a large number of elements that are meshed on empty space, i.e. they are elements which contain no solid material. This means that a much higher number of elements is required to converge to an

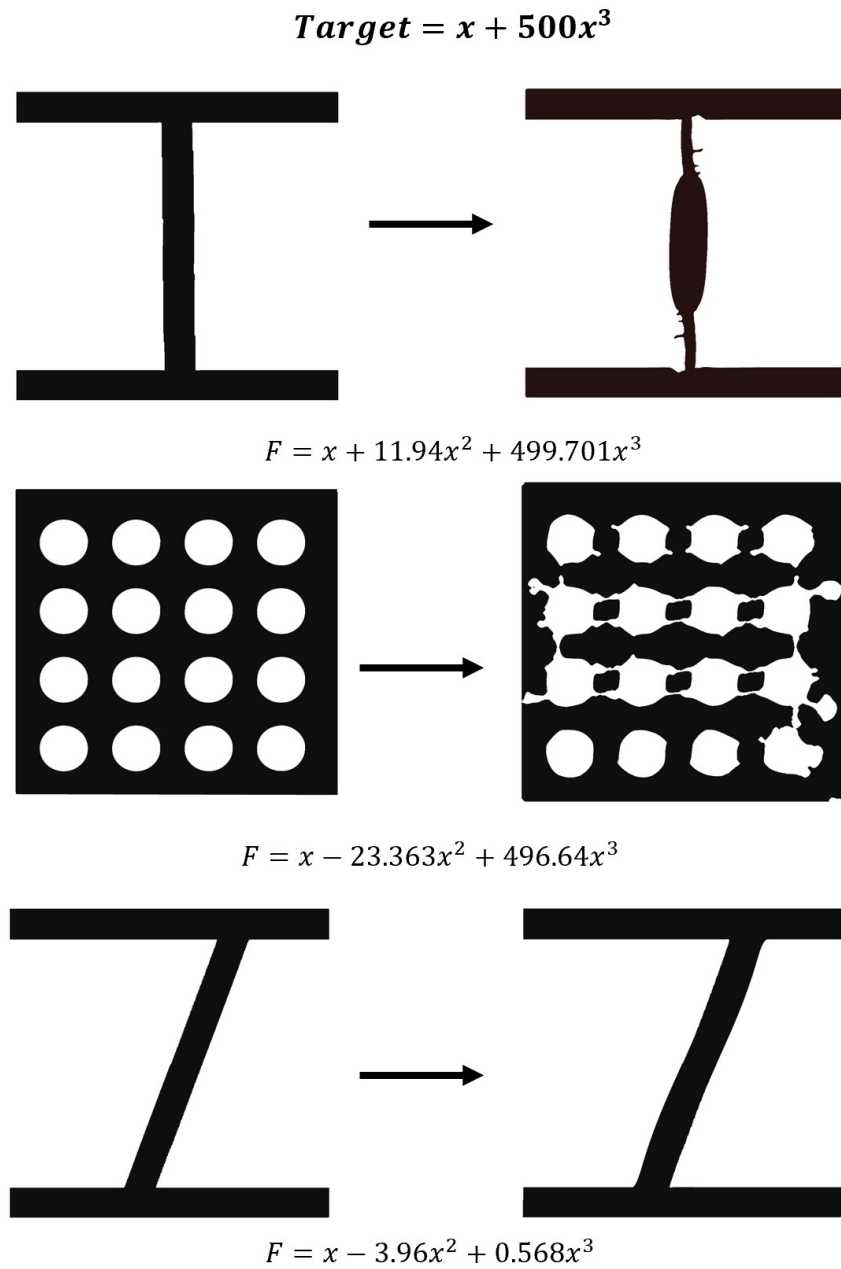


Figure 2.7. A coarsely meshed exploration of the effect of initial condition upon final design and achievable performance. The domain is fixed along the top edge, fixed in the vertical direction along the bottom edge (rollers), and pulled to the right from the bottom right corner.

accurate solution as compared to the COMSOL body-fitted mesh, which covers only the areas which contain material.

Table 2.2. Mesh Sizing Details

Target Polynomial (Normalized)	Optimization Final Mesh Size	COMSOL Verification Number of Elements
$x + 163.3x^3$	580 x 580	91,397
$x - 40.0x^3$	580 x 580	66,637
$x + 28.887x^2 - 278.135x^3$	750 x 750	58,904
$x - 12.380x^2 + 119.196x^3$	700 x 700	80,451
$x - 10.0x^2 + 30.004x^3$	700 x 700	33,846
$x + 120x^3$	580 x 580	43,588
$x + 80x^3$	580 x 580	70,652
$x + 40x^3$	580 x 580	57,437
$x + 20x^3$	580 x 580	60,180
$x + 10x^3$	580 x 580	66,924
$x - 41.064x^2 + 396.11x^3$	750 x 750	28,442
$x + 200x^2 + 0x^3$	700 x 700	28,576
$x + 150x^3 - 150x^4$	650 x 650	23,715

2.4.3 Cubic sweep full structures

We include here in Fig. 2.11 the full set of the optimized structures for the linear plus cubic stiffening sweep shown in Fig. 2.5 in the main text.

2.4.4 Linear solver details

We note the use of the parallel linear solver HSL MA97 in the nonlinear FE problem.

[159]



Figure 2.8. The initial conditions used for the softening (top left), stiffening (top right), softening to stiffening (bottom left) and stiffening to softening (bottom right) optimizations. The boundary conditions imposed on the softening, stiffening, and softening to stiffening cases are: 1) fixed along the top edge, 2) roller along the bottom edge, and 3) applied displacement along the lower right edge. The boundary conditions imposed on the stiffening to softening case are: 1) fixed along the left edge and the top right corner, 2) roller along the bottom edge, and 3) applied displacement along the lower right edge.

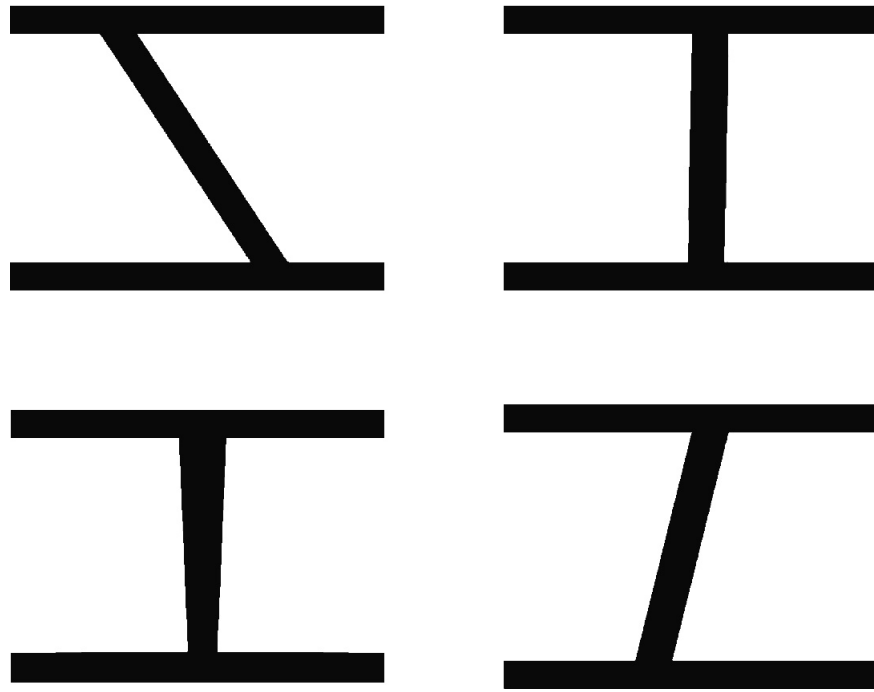


Figure 2.9. The initial conditions used for the quadratic stiffening (top left), bistable (top right), fourth order (bottom left) and negative stiffness (bottom right) optimizations. The boundary conditions imposed on all cases are: 1) fixed along the top edge, 2) roller along the bottom edge, and 3) applied displacement along the lower right edge.



Figure 2.10. The initial condition used for the cubic sweep ratio 20 optimization. The boundary conditions imposed are: 1) fixed along the top edge, 2) roller along the bottom edge, and 3) applied displacement along the lower right edge.

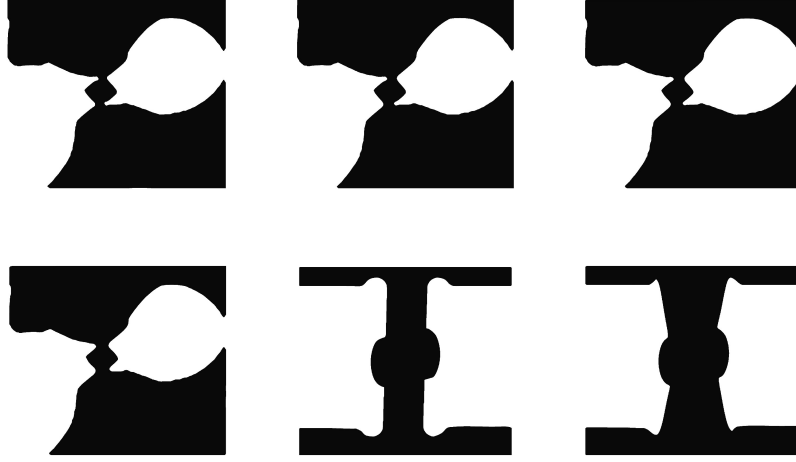


Figure 2.11. The full optimized structures from the linear plus cubic sweep. Top row, left to right: ratio 163, ratio 120, ratio 80. Bottom row, left to right: ratio 40, ratio 20, ratio 10.

2.4.5 Excessive Distortion of Soft Elements

The excessive distortion of soft elements is a well known issue in large deformation FEM problems. Due to the use of a fixed mesh in this work, and the meshed elements in the empty space being approximated as very soft elements with near zero stiffness, the examples run in the main text have a large number of soft, highly deformable elements which could potentially excessively deform, which could lead to poor FEM solver convergence. Most examples in the main text were run without encountering such issues. However, the problem tends to arise more frequently in geometries with sharp angles and small hinge-like structures, such as Fig. 2.5B and 2.3D in the main text, which did encounter issues with solver convergence. An examination of the element-level deformation gradient,

$$F_{ij} = \frac{\partial x_i}{\partial X_j}, \quad (2.3)$$

wherein x represents the deformed coordinates and X represents the reference coordinates, provided confirmation of excessive element deformation. When the determinant of the element

deformation gradient becomes negative, it is an indication that the current deformed mesh has deformed to the point that the transformation between the reference and deformed coordinates results in a negative area or volume (*i.e.* a non-physical transformation).

In cases where this excessive deformation caused impedance to accurate convergence to a solution (namely, example 2.3D), a method was implemented to remove the bulk of the soft elements from the solution process, thus improving convergence. Nodes that were more than a critical threshold away from the boundary (in this case, a level set value of -3 was chosen) were assumed to have force and displacement values of 0, and were removed as free degrees of freedom from the problem. Thus, the Newton-Raphson solver dealt with a reduced degree of freedom problem (in which the reduced degrees of freedom were updated for every optimization iteration, as the shifting level set boundary shifted which nodes were included in the exclusion zone). We note that this approach introduces inaccuracies within the ‘transition’ elements (the elements which have a portion of their nodes over the threshold and a portion of them not). For large deformation theory, the Green-Lagrangian strain tensor (used in the nonlinear finite element equations herein) is defined as $E = \frac{1}{2}(C - I)$, in which I is the identity matrix, and C is the Cauchy strain tensor, defined as $C = F^T F$. As $x = X + u$, an assumed value of $u = 0$ therefore alters the internal strain and stress tensors of the element, leading to inaccurate element-level internal force and stiffness values. The choice of the cutoff threshold at -3 addresses this by ensuring that there is a ‘buffer’ of soft elements (whose solution we do not particularly care about) around the meshed structure (whose solution we do care about). The ‘transition’ elements where these inaccuracies are introduced are, therefore, entirely soft elements. As the element force and stiffness values are scaled by the element area fraction ($1e^{-9}$ in the case of fully soft elements), these inaccuracies have a negligible effect upon the solution.

The accuracy of the approach was verified by comparing the optimizer solution from Fig. 5B, which used the above described framework, with the same design simulated in COMSOL. The results are shown in Fig. 2.12.

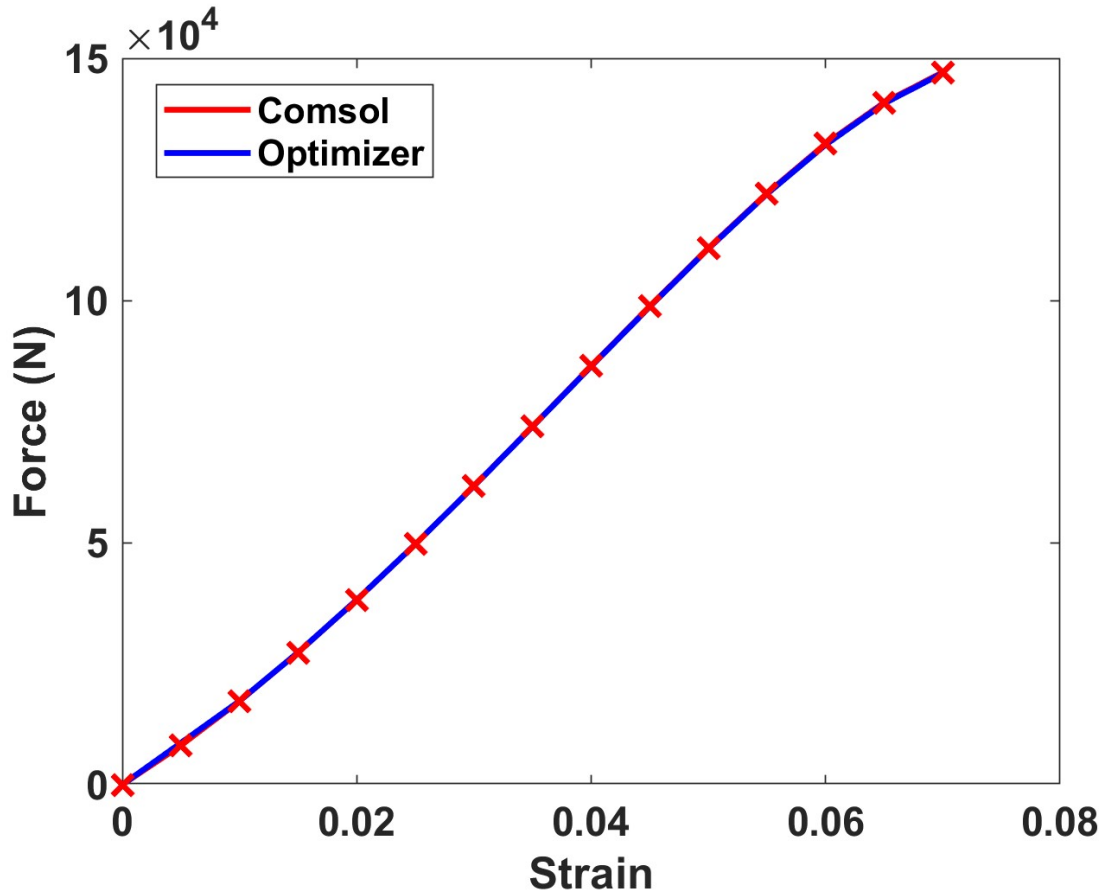


Figure 2.12. Validation of the method used to cut out excessively deforming elements, comparing the solution from the optimization code FEM (blue line) with the same design simulated in COMSOL (red line with red x markers).

2.4.6 Experimental validation and sample manufacturing details

In order to validate the optimized designs, the optimized structures were fabricated and tested quasi-statically upon an MTS tensile tester, and the performance was compared to the computationally calculated force-displacement performance. The fabricated designs consisted of a frame with structural rigidity significantly greater than that of the spring itself, used to ensure equivalent boundary conditions as the FE model, and two or four (in the case of the bistable design) of the optimized spring structures. The two optimized structures were mirrored across the edge of the design domain with the roller boundary condition (the bottom edge, as represented in the figures herein and in the main text), as this roller boundary condition represents a line of

symmetry. A sketch of this design is shown in Fig. 2.1E.

The optimized design level set functions were exported from the optimization code, and x and y coordinates were fit to the level set boundary. These x and y coordinates were then imported into Abaqus as a spline fit, using Abaqus Python scripting, in order to create a usable 2D sketch of the optimized structure. From there optimized structures were exported as parts, analyzed through finite element analysis in COMSOL Multiphysics (as described above), and final fabrication files were assembled in SolidWorks.

Samples were then physically fabricated with one of two different methods, depending upon the material out of which the sample was constructed. For designs which were thin enough to utilize the Kirchhoff material model without inducing plasticity in the course of the applied displacement, the designs were fabricated out of polycarbonate. The stiffening-to-softening sample was cut from a polycarbonate square in a single piece, using a CNC machine. The spring was cut to a greater depth than the frame ($1/8$ inch), resulting in a thicker frame ($1/4$ inch), designed to increase stiffness and minimize flexing of the frame during the applied spring deformation, in order to enforce fixed boundary conditions. The bistable spring proved to be more sensitive to boundary conditions, and so the spring portion was cut from a thin piece of polycarbonate ($1/8$ inch), while the frame was manufactured out of stainless steel in order to increase its stiffness beyond that achievable by a polycarbonate frame, for a better enforcement of the rigid boundary conditions. In this case, the polycarbonate spring was carefully sanded down to fit within the external steel frame, and was attached to the frame via an acrylic back plate, which was screwed into the frame and glued to the polycarbonate boundary of the spring (see Figure 2.13.) Furthermore, the bistable spring utilized four optimized spring structures, rather than the two used in other cases, in order to reduce the tendency to buckle out of plane during snap-through. For designs which were too thick to utilize the Kirchhoff material model, and instead used a Neo-Hookean material model, the springs were fabricated out of Zhermack Elite Double 32 silicone. Molds were cut from acrylic using a laser cutter. In order to accommodate the simulated plane strain conditions, several layers of acrylic were glued together to construct

a deeper mold and frame, such that the samples were thicker in the depth direction than in the width and height directions.

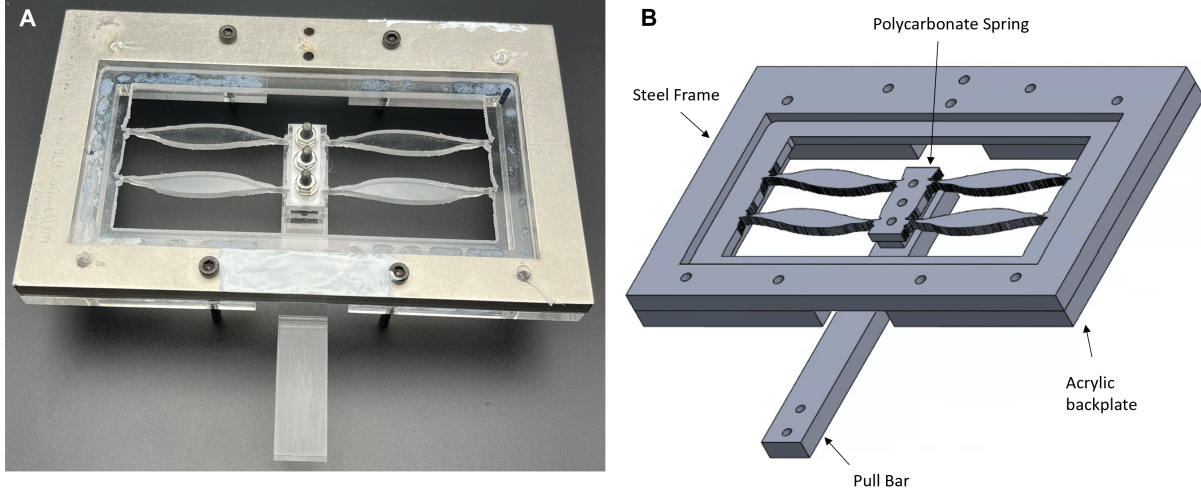


Figure 2.13. The integrated spring-frame design of the bistable spring, used for quasi-static validation testing. A) a photograph of the final manufactured spring. B) A CAD model of the spring-frame assembly.

We note that, in addition to the straightforward scaling performed between simulation dimensions and experiment dimensions described in the main text, the experimental data requires a shift in the equilibrium point (the point which passes through zero force and displacement) in order to account for shifting of equilibrium induced by the weight of the spring and the process of clamping the sample into the testing machine. Additionally, there existed some level of uncertainty in the modulus used to convert between simulation and experiment data sets, which may result in an offset in the vertical scaling direction, but does not impact the shape of the nonlinearity. In the case of the silicone designs, this was due to the observed continual curing of the silicone over a period of several weeks after spring fabrication. In the case of the polycarbonate, this was due to manufacturing constraints (specifically, the CNC bit radius), which prevented exact accuracy in cutting sharp corners, thus introducing extra stiffness. The modulus value used for the scaling described in the main text was therefore selected based upon the difference in the maximum force between the simulations and the experiments.

The dimensions of the fabricated springs, used for scaling, are as follows. The bistable polycarbonate spring had a thickness of 3.175 mm, and a unit cell length of 59 mm. The softening to stiffening silicone spring had a thickness of 23.5 mm, and a unit cell length of 50.05 mm. The stiffening to softening polycarbonate spring had a thickness of 3.175 mm, and a unit cell length of 38.1 mm.

2.5 Acknowledgements

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Chapter 3

Customizable wave tailoring materials enabled by coupling nonlinear inverse design at two scales

Passive transformation of waves via nonlinear systems is ubiquitous in settings ranging from acoustics to optics and electromagnetics. Passivity is of particular importance for responding rapidly to stimuli and nonlinearity enormously expands signal transformability compared to linear systems due to the breaking of superposition. It is well known that different types of nonlinearity yield vastly different effects on propagating signals, which raises the question of “what precise nonlinearity is the best for a given wave tailoring application?” Considering a one-dimensional spring-mass chain as a testbed, we couple the shape optimization of structures for tailored nonlinear constitutive responses with reduced-order nonlinear dynamical inverse design. Using minimization of peak kinetic energy transmission from impact as a case study, we identify ideal nonlinear constitutive responses and the geometries needed to achieve them. As part of this, we show the large sensitivity of this metric to small changes in nonlinearity, and thus the need for high precision, free-form nonlinearity tailoring. We validate our predictions using impact experiments in a chain of nonlinear springs and masses. This work sets the foundation for broader passive nonlinear mechanical wave tailoring material design, with applications to computing, signal processing, shock mitigation, and autonomous materials.

3.1 Introduction

The passive transformation of waves via nonlinear material response is widely used in physical settings ranging from acoustics [76] to optics [160–162] and electromagnetics [163, 164]. Applications include areas such as efficient information transfer [165, 166], computing and logic [167, 168], energy conversion [169], imaging [170], encryption [171], impact and vibration mitigation [172, 173], and rapid shape change [174]. Within these contexts, in contrast to active control, passivity is of particular importance for responding fast to stimuli, and nonlinearity enormously expands signal transformability compared to linear systems due to the breaking of superposition. Indeed, it is well known that different types of nonlinearity yield vastly and qualitatively different effects on propagating signals [175], which raises the question of “what precise nonlinearity is the best for a given wave tailoring application?” This question has largely remained in the regime of simulation and theory, as, until recently, it has not been possible to freely realize any optimal nonlinear constitutive law in practice. The field of mechanics has come furthest towards this goal, by introducing complex, sub-wavelength, geometric motifs to create “mesostructured” nonlinear materials [76], however any tunability seen has been limited around a handful of known nonlinear mechanisms. For instance, broad classes of nonlinearity that have seen tailorability for wave manipulation include contact nonlinearities [147], tensegrity structures [25], and bistable beam arrays [176], among others.

Recent progress has enabled a, thus far unique-to-mechanics, capacity to create materials with on-demand quasi-static nonlinear properties via shape and structural optimization [22, 23, 62, 64, 152, 177–179]. This has included several approaches, including gradient based topology optimization in pursuit of tailoring the entirety of a nonlinear force-displacement curve [22, 62, 177] as well as the incorporation of machine learning (ML) algorithms in an attempt to traverse the design space and speed up predictions of mechanical behavior [23, 24, 64, 152, 179]. However, such methods alone cannot identify material designs for optimal system-level nonlinear wave tailoring performance. Prior studies of optimal nonlinear dynamic material behavior have

tailored heterogeneity with fixed nonlinearity [180], or dynamic behavior where the characteristic wavelengths are on par with or greater than the system size (and thus the response is not “wave-dominated”) and the tailoring was confined to broad metrics like “area under the curve” [20, 66] or “plateau-like” behavior [67]. The role of waves is of particular importance, as allowing for spatiotemporal evolution in nonlinear systems leads to unique emergent phenomena such as solitons [181]. The role of precisely engineered nonlinearities is further important for wave propagation in that seemingly subtle differences in nonlinearity yield *qualitatively* different dynamical behavior. For one example, consider a material with polynomial nonlinearity and all positive coefficients, resulting in a “stiffening” nonlinearity: just small changes in the ratio of coefficients dictate whether or not the system experiences modulational instability [182, 183], or the difference of a quadratic versus cubic perturbation on a linear stiffness results in qualitatively different waveforms and wave mixing behavior [160]. Connecting the inverse design of nonlinear wave response to the quasi-static design of nonlinear constitutive response induced by mesostructure geometry is a significant, and hitherto unsurmounted challenge. If trying to directly extend quasi-static geometric design algorithms based on finite element method (FEM) simulation [22, 23, 62, 64, 152, 177–179] the challenge becomes evident, in that one would need to take the same design variables, copy the geometry over many unit cells, and simulate the entire system in time at high temporal resolution (due to nonlinear generation of high frequency content), and wrap that in an automated design loop—resulting in a task of extreme computational expense.

In this work, we introduce a method to create customizable wave tailoring materials via nonlinear bilevel inverse design. Namely, we optimize for the emergent dynamic response of a mesostructured material in the form of a one-dimensional (1D) spring-mass chain. To do this, we use a reduced order, discrete element model (DEM) simulation to identify an optimal nonlinear constitutive law for the given performance metric, and couple this to a unit-cell-scale, geometrically-nonlinear, free-form, shape optimization algorithm which designs a physical system that achieves the nonlinear constitutive property identified by the DEM

(outlined in Fig. 3.1). We note that the 1D spring-mass chain is a prototypical nonlinear system that has classically formed the foundation for extensions into higher dimensions and continua [175, 181, 184], and, as part of our work herein, we illustrate extensions of our optimized unit-cells to two- and three-dimensional analogs (see Supplementary Information Note 1). Further, we demonstrate the clear need for high precision nonlinear response design, wherein the system dynamic performance is shown to be highly sensitive to the nonlinear coefficients of the constitutive law. Herein, we choose the maximum kinetic energy transmitted to the boundary of the system in response to an impact event, normalized by that of an otherwise-identical linear system, as our performance metric. The comparison between the linear and nonlinear response is particularly important, as it isolates the role of nonlinearity from other wave manipulating effects such as dispersion and dissipation. We demonstrate the full inverse design of this superior impact mitigation system, from identification of an ideal nonlinearity, to the design of the unit cell geometry, and experimental validation of the performance. An important feature to note, unlike some prior computational quasi-static nonlinear mechanical design strategies [22, 23, 65, 178], we do not use simplified or reduced order models for our underlying mesostructure design, which enables a broader design space and access to highly precise tailoring of nonlinear responses [177]. While we demonstrate our bilevel inverse design for the case of impact mitigation, we expect such an approach for the previously specified nonlinear wave transformation applications [76, 165–171] within the acoustic, phononic, and mechanical wave settings.

3.2 Results

3.2.1 Reduced order discrete element model

The DEM (Fig. 3.1A) simulates the impact of a rigid “impactor” block onto a chain with N unit cells and a unit cell length. We represent the chain as lumped masses of mass m , interconnected by massless nonlinear springs and inter-site linear dampers in parallel, emulating the behavior of a viscoelastic material. The nonlinear spring consists of a linear spring behavior

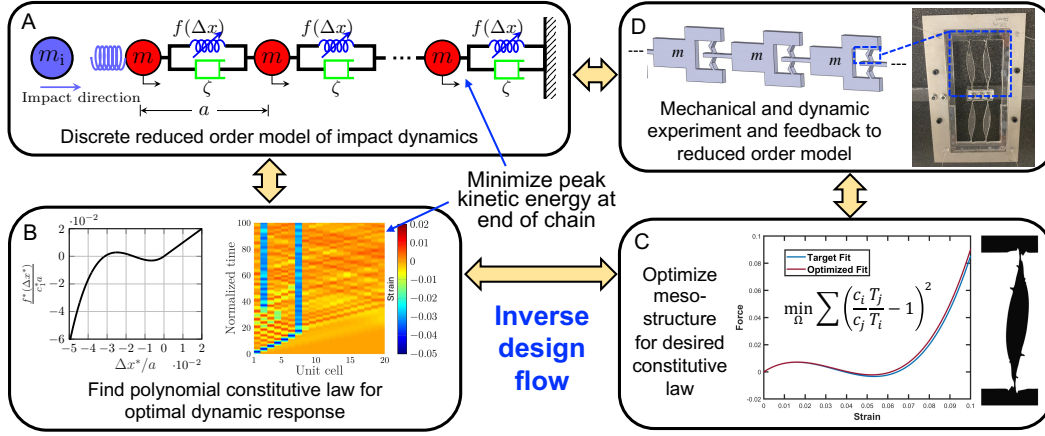


Figure 3.1. Overview of the bilevel design flow. (A) Discrete element model (DEM) simulation of the entire system dynamics. (B) Identification of the optimal nonlinear constitutive law. (C) Shape optimization of a mesostructure to match the identified nonlinear constitutive law. (D) Mechanical and dynamic experimental system characterization.

in tension and an up-to-third-order polynomial in compression, where the linear stiffness remains fixed at c_1^* in both tension and compression (as shown in Fig. 3.1B). This results in non-dimensionalized equations of motion for our chain

$$\ddot{x}_i - (x_{i+1} - x_i) + c_2(x_{i+1} - x_i)^2 - c_3(x_{i+1} - x_i)^3 + (x_i - x_{i-1}) - c_2(x_i - x_{i-1})^2 + c_3(x_i - x_{i-1})^3 + 2\zeta(-\dot{x}_{i+1} + 2\dot{x}_i - \dot{x}_{i-1}) = 0, \quad (3.1)$$

where dimensionless stiffnesses c_2 and c_3 are zero when that spring is in tension, ζ is the inter-site damping ratio, x_i is the dimensionless displacement of the i th particle from its rest position, overdots represent the derivative with respect to nondimensional time, and all variables and parameters are normalized by combinations of a , m , and/or c_1^* , as is described in Supplementary Information Note 2. We note that while the masses are illustrated as m in Fig. 3.1A, the nondimensional mass of each particle remains one as in Eq. (3.1). A variable mass and velocity rigid impactor is applied on the left, and a fixed boundary on the right. The model also incorporates a contact spring designed to facilitate the smooth contact and controlled release of the impactor during initial impact and rebound, respectively. The simulated dynamical response

is acquired through the numerical integration of Eq. (3.1) via a Runge-Kutta algorithm. The non-dimensionalization of all variables and full details concerning the equations of motion are described in Supplementary Information Note 2.

3.2.2 Optimization of nonlinear constitutive law based on dynamical response

Before searching for optimal nonlinear constitutive responses with our DEM, we set several bounds. First, we confine the unit cell strain to 1 in compression, and set $c_3 > 0$ for simplicity. Second, we restrict our search range for nonlinear coefficients c_2 and c_3 to ensure positive strain energy throughout the entire compression range. We note that keeping the linear stiffness constant, we exclude essential nonlinearities [172]. By examining the polynomial's properties within this range, we classify the quasi-static response into three distinct zones, “bistability”, “monotonic increase”, and “local maximum”, as shown in Fig. 3.2A. Bistability (magenta area) denotes the existence of both a local maximum and minimum other than the boundaries (the local minimum does not need to fall below zero). Monotonic increase (blue area) denotes the absence of extrema. Local maximum (green area) signifies the presence of a local maximum (no local minimum existed) within the range of the length of one unit cell. More details concerning these zones is given in Supplementary Information Note 3.

Within these bounds, we first optimize for a singular impact condition ($M/M_0 = 0.05$ and $V/V_0 = 1$), where M_0 is half the mass of the chain, V_0 is the linear sound speed, and M and V are the dimensional impactor mass and velocity, respectively. The material is composed of 20 particles and $\zeta = 0.01$. We vary the nonlinear coefficients of the springs c_2 and c_3 , aiming to minimize the maximum kinetic energy experienced at the end of the material (KE_{non}) normalized by that of a linear system (KE_{lin}) which has all of the same properties except $c_2 = c_3 = 0$. Given dimensional particle displacement from its rest position x_i^* , kinetic energy of the i th particle is defined as $m(dx_i^*/dt^*)^2/2$, where t^* is dimensional time, such that the analogous dimensionless kinetic energy is $\dot{x}_i^2/2$. Figure 3.2C quantifies the ratio of maximum kinetic energy at the

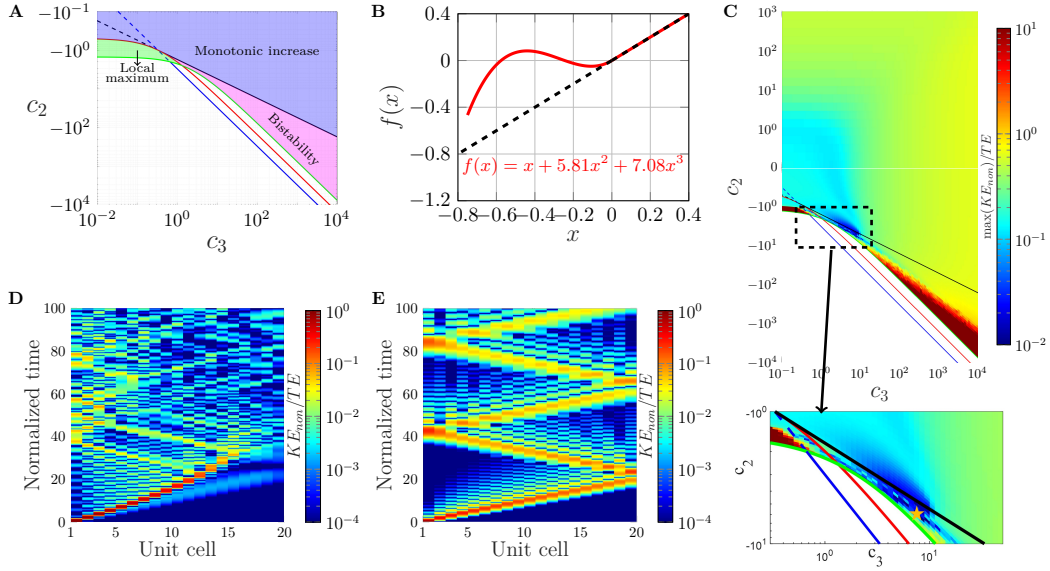


Figure 3.2. Identification of optimal nonlinear constitutive response via DEM simulation for a single impact condition. (A) Feasible solutions of nonlinear spring coefficients c_2 and c_3 . The black line represents $c_2 = -\sqrt{3c_3}$, the red line indicates $c_2 = -(1 + 3c_3)/2$, the blue line is $c_2 = -3c_3$, and the green line is the zero strain energy throughout the whole range, $c_2 = -3/2 - 3c_3/4$. (B) Non-dimensional force displacement relationship of the best performance of the nonlinear spring. (C) Ratio of maximum kinetic energy at the last particle in the nonlinear chain to the initial impact energy as a function of nonlinear spring coefficients for the impact condition of $M/M_0 = 0.05$ and $V/V_0 = 1$, as well as $\zeta = 0.01$. The lines from (A) are overlaid, and the star marker denotes the point of best performance. Normalized kinetic energy of the (D) best performing nonlinear and (E) linear material.

end of the material to the initial impact energy (TE), as a function of the coefficients of the nonlinear spring. The best performance in Fig. 3.2C corresponds to nondimensional spring force $f(\Delta x) = \Delta x + 5.81\Delta x^2 + 7.08\Delta x^3$, where Δx is the spring extension and positive f denotes tension. This optimal spring is plotted in Fig. 3.2B, and is denoted by the star marker in the inset of Fig. 3.2C. A point of particular note about this identified optimum, is that it is not of the form one would expect based on the conventional design approach for bistable energy absorption at lower rates [185], where net positive energy is locked into strain energy when snapping from the undeformed state to its second stable equilibrium (*i.e.*, the area under the curve from $\Delta x = 0$ to the unstable equilibrium point (at $\Delta x \approx -0.2$), is less than the area under the curve from the unstable equilibrium to the second stable equilibrium point (at $\Delta x \approx -0.6$).

Rather in the case of our optimum, the first area is smaller than the second. Around this point of best performance, significant performance sensitivity to the constituent nonlinear parameters can be seen (see the zoomed-in view in Fig. 3.2C). To describe this sensitivity more quantitatively, in Supplementary Information Note 4 we calculate the gradient of the inset in Fig. 3.2C, which shows $\partial(\log_{10}(KE_{non}/TE))/\partial c_2$ and $\partial(\log_{10}(KE_{non}/TE))/\partial c_3$ approaching ± 10 . This metric thus suggests that, *e.g.*, a 0.1 difference in c_2 or c_3 can result in up to a $10\times$ change in peak KE . However, we emphasize that near our chosen optimum, the sensitivity is significantly lower, with $\partial(\log_{10}(KE_{non}/TE))/\partial c_2 = 0.32$ and $\partial(\log_{10}(KE_{non}/TE))/\partial c_3 = 0.07$. Spatiotemporal responses of kinetic energy of the optimal nonlinear and linear chain are shown in Fig. 3.2(D) and (E), respectively. In Fig. 3.2(D) and (E), while both materials exhibit an initially sharp pulse, energy from the optimal nonlinear material is trapped around particle 15, preventing further transmission.

In the subsequent analysis, we conduct an optimization wherein we look for optimal nonlinear coefficients for varied impactor mass and velocities. We use the same ratio of the maximum KE of the last particle of the nonlinear material normalized by that of the linear material as a performance metric (denoted henceforth as “ KE ratio”), wherein a lower ratio indicates superior performance of the nonlinear material. The optimal (minimum) KE ratios with respect to M/M_0 and V/V_0 and corresponding nonlinear spring parameters c_2 and c_3 can be seen in Fig. 3.3. In contrast to Fig. 3.2, we use lower damping ($\zeta = 0.005$), chosen to emulate that of the polycarbonate springs used in our experimental realization. Additional simulation results of KE ratios for increased damping and greater discreteness (more unit cells) are available in Supplementary Information Note 5 and indicate the potential for KE ratio $< 10^{-2}$ in the latter case. The damping value used in Fig. 3.3 was chosen by measuring the low-amplitude resonance of a single connector and nonlinear spring unit (see Supplementary Information Note 6). This is an important point to highlight, in that the characterizing the damping at low amplitudes allows us to temporarily discard its interplay with the nonlinear spring. This damping can be thought to stem from the intrinsic damping of the polycarbonate. Using the model of the nonlinear spring

with the linear damper in parallel, thus allows us to simulate greater effective damping that may come from their dynamical interplay at higher amplitudes. Simulation cases of the nonlinear material where self-contact occurs are discarded from consideration of the optimal performance.

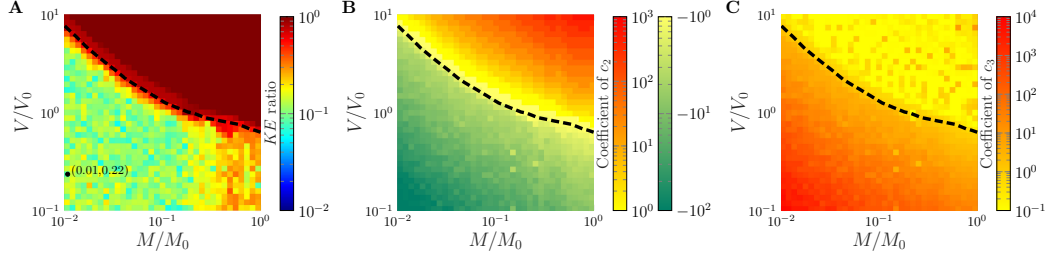


Figure 3.3. Identification of optimal nonlinear coefficients via DEM simulation for varied impactor conditions. (A) Optimal kinetic energy ratio (KE ratio) as a function of impact conditions and corresponding nonlinear spring coefficients (B) c_2 and (C) c_3 for a material of $N = 20$ and $\zeta = 0.005$. The color bar in (A) is saturated at a KE ratio of unity. The dashed black line denotes the onset of self contact ($x < -1$) in the linear system. The dot in (A) denotes the high performing case used for mesostructure design.

There is a clear boundary where the nonlinear chain does not outperform the linear, which is correlated with the occurrence of self-contact within the linear chain (dashed black line in Fig. 3.3). At impactor velocities and masses below this threshold, the nonlinear materials exhibit significantly enhanced mitigation effectiveness. As can be seen in Fig. 3.3A, at a relatively low to moderate level of impactor mass (~ 0.01 to $0.2M_0$), optimal nonlinear materials exhibit a mitigation capability (KE ratio) that is over ten times better than the linear material. As the impactor mass and velocity increase and cross over the dashed black line (orange to red area near the dashed line in Fig. 3.3A), the priority shifts to preventing contact between unit cells, leading to a comparatively impaired energy-absorbing performance. In future studies, such self contact could be explored as a form of nonlinearity, and a design feature instead of a constraint.

A specific optimal solution (pair of coefficient ratios) was chosen from a set of multiple solutions showing high performance KE ratio. We further downselected, looking for a solution also with relatively low strain, making it more amenable to experimental implementation. The chosen solution is a nondimensional nonlinear mechanical response of the form $f(\Delta x) = \Delta x +$

$87\Delta x^2 + 1778\Delta x^3$ in compression, with an impact condition of $M/M_0 = 0.01$ and $V/V_0 = 0.22$ (marked in Fig. 3.3A). This nonlinear constitutive law is used as the target for the mesostructure design, with the goal of finding a geometry that yields that nonlinear mechanical response.

3.2.3 Shape optimization for desired nonlinear constitutive law

In order to find a spring geometry that gives the desired nonlinear response, a two-dimensional shape optimization approach is taken, using a level-set optimization method (as detailed further in the Methods and Ref. [177]). In summary, a third order polynomial is fit to the calculated force-displacement behavior of the structure, and the objective of the optimization problem is taken as the ratio of nonlinear to linear terms (*e.g.*, as shown in Fig. 3.1C and Fig. 3.4A). The exact form of the objective function is

$$\min_{\Omega} \sum \left(\frac{c_i}{c_j} \frac{T_j}{T_i} - 1 \right)^2, \quad (3.2)$$

where c_i and c_j represent the current polynomial coefficients, and T_i and T_j represent the target coefficients. By taking the ratio of the polynomial terms, the nonlinearity of the structure is decoupled from the linear stiffness, allowing the optimizer more design freedom, leading to more robust convergence. To further aid in the navigation of the design space, we select an initial condition for our optimization process, which displays qualitatively similar behavior to that desired (see Supplementary Information note 6).

The boundary conditions applied are depicted in Fig. 3.4B (fixed on top, roller on bottom, applied displacement on bottom 10% of the right boundary). When realizing our nonlinear chain, we employ comparatively rigid frames around the designed spring to mimic fixed boundary conditions (as can be seen in Fig. 3.1D and Fig. 3.4C) and rigid connectors between the springs to allow relative movement of the masses. With the addition of these components we have a unit cell length, a , and a nonlinear spring design domain length that encompasses only a portion of this larger unit cell. We call this portion of a the spring length, and denote it by a_s (and,

hereafter, the subscript s is used to refer to parameters defined on the scale of the spring). Figure 3.4E highlights the difference between these two length scales. Because the DEM-identified polynomial constitutive law is expressed as a function of strain, and the strain experienced by the spring across a_s is different than that experienced by the entire unit cell across a for a fixed applied displacement, the targeted polynomial is therefore scaled accordingly. We take the ratio of nonlinear terms as $R = (c_i \epsilon^i) / (c_1 \epsilon)$ and $R_s = (c_{s,i} \epsilon_s^i) / (c_{s,1} \epsilon_s)$ on the scales of a and a_s , respectively, with i representing the order (or power) of the term and ϵ representing the maximum strain experienced on the corresponding length scale. In order for equivalent degrees of nonlinearity to be displayed at different scales, we take $R = R_s$ at the maximum strain considered in each scale, and solve for updated c_i or $c_{s,i}$ terms.

The optimization target (recall, on the unit cell scale, identified above as $f(\Delta x) = \Delta x - 87\Delta x^2 + 1778\Delta x^3$) can therefore be expressed on the spring length scale as $f(\Delta x_s) = \Delta x_s - 41.064\Delta x_s^2 + 396.11\Delta x_s^3$, by setting $R = R_s$ and solving for $c_{s,i}$. The final optimized structure, shown in Fig. 3.4A-B, achieved a simulation force-displacement law on the spring scale of $f(\Delta x) = \Delta x_s - 40.712\Delta x_s^2 + 397.535\Delta x_s^3$, and an experimental one of $f(\Delta x) = \Delta x_s - 40.654\Delta x_s^2 + 397.274\Delta x_s^3$ (shown in Fig. 3.4D), resulting in an experimental percent difference between targeted and obtained polynomial ratios of 0.294% for the third order ratio and 0.998% for the second order ratio.

As the multilevel optimization methodology is a loop, in which inputs from the DEM and shape optimization feed back into one another, the design process can be followed in either direction, which can be exploited for exploration of the space. For example, while one may begin with a desired impact condition, which is then fed into the DEM simulation followed by the mesostructure optimization, one might just as easily begin with some nonlinearity and feed this into the DEM simulation to explore what impact conditions it might perform well (or poorly) for. Similarly, one might find that the physical design domain requires constraints, or that optimized structures exhibit structural damping, which diverges significantly from predictions, and these updated considerations can be flowed back up to the DEM simulation to search for the updated

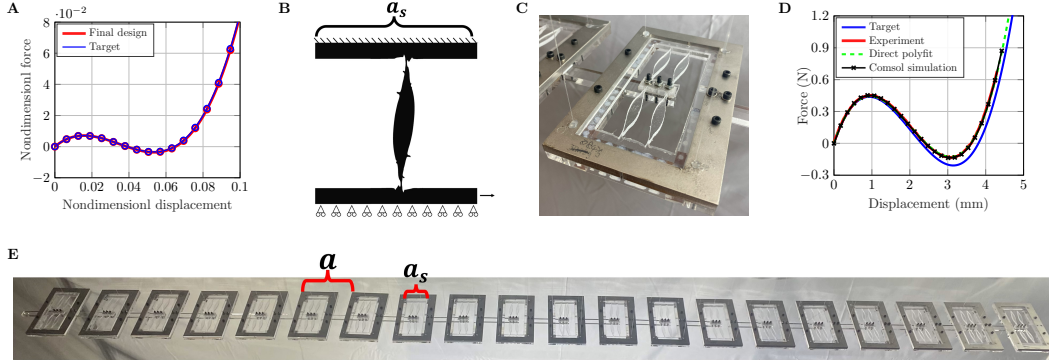


Figure 3.4. Shape optimization to identify geometry giving DEM identified desired constitutive law, and experimental realization of the spring and chain. A-B) Results of the shape optimization, with the target and final force-displacement curves shown in (A), and the optimized design shown in (B). C) The fabricated polycarbonate unit cell, consisting of four optimized springs (as seen in (B)) and a rigid frame to impose boundary conditions. D) The quasi-static test of the unit cell shown in (C), compared against the behavior of a single spring with perfectly imposed boundary conditions as simulated via COMSOL FEM simulation. E) The full chain of 20 unit cells, hung from a frame. The chain is clamped to the left of the leftmost unit cell, imposing a zero displacement boundary condition. The impact occurs at the right end of the chain. The unit cell and spring length scales are labeled.

optimum conditions.

In the example shown herein, we strive for generality, thus there was no single impact condition specified. The solutions were chosen which exhibited low impactor mass and velocity, relatively smooth sensitivity to impact conditions (discussed in more detail below), and low maximum strain in order to avoid the onset of plasticity in the fabricated structures. One can just as well begin with a strict impact condition requirement, and flow through the multilevel optimization methodology accordingly. If larger mass and velocity, and therefore larger strains, are desired, the mesostructure optimization portion can be undertaken with a Neo-Hookean material model, and the real-world structures fabricated out of some soft, flexible material, such as silicone (see Ref. [177]).

3.2.4 Experimental validation

In our experimental realization of the chains, the spring scale $a_s = 59$ mm was chosen and incorporated into the rigid frame and connector, resulting in a unit cell length $a = 125$ mm. A

chain of twenty unit cells (a single unit cell is shown in Fig. 3.4C) was fabricated and hung from a frame in order to minimize friction, as shown in Fig. 3.4E (see Note 7 in the Supplementary Information for a more detailed breakdown of the chain design). Impact tests were undertaken where the mass and velocity of the impactor were chosen based upon the optimal conditions identified in the DEM results, in the case with an impactor mass of $M = 40$ g and a velocity of $V = 1.37$ m/s. Data was collected through the use of several cameras positioned along the length of the chain, allowing digital image processing to be used to track the impact wave across the length of the system. In addition, a laser Doppler vibrometer (see Supplementary Information Note 7) was pointed at the last unit cell in the system, allowing for a second measurement of the velocity of the last unit cell. Impact tests were repeated several times. A similar chain of twenty linear unit cells, with similar linear stiffness and mass (the mass of the linear and nonlinear unit cells are 400.4 g and 398.8 g, respectively) values, was then constructed to act as a control for comparison against the nonlinear chain (see Supplementary Information Note 6 for more details), and the impact tests were repeated. It is noted that for the kinetic energy transmission ratio considered herein, the magnitude of the linear stiffness (even if different between the linear and nonlinear chain) does not matter (see Supplementary Information Note 8).

Several key metrics were examined to confirm the performance of the system, the results of which are summarized in Fig. 3.5. Foremost among these results is the velocity (or kinetic energy) which was transmitted to the end of the chain. Measured spatiotemporal kinetic energy responses are shown in Fig. 3.5A-D, in which we can see that the nonlinear cases dissipate and trap kinetic energy through unit cell snapping, preventing much of it from reaching the right (or protected) end of the chain (a large portion of the kinetic energy is seen to remain, reflecting back and forth, in the first 9-11 unit cells in panels A and B). We note an excellent match between simulation (using the experimentally fit coefficients taken from the quasi-static force-displacement curve shown in Fig. 3.4D) and experiment in these spatiotemporal plots. Figure 3.5E shows a comparison of the ratio (of linear to nonlinear cases) of the maximum kinetic energy seen at each unit cell, in both experiment (averaged across three trials) and simulation.

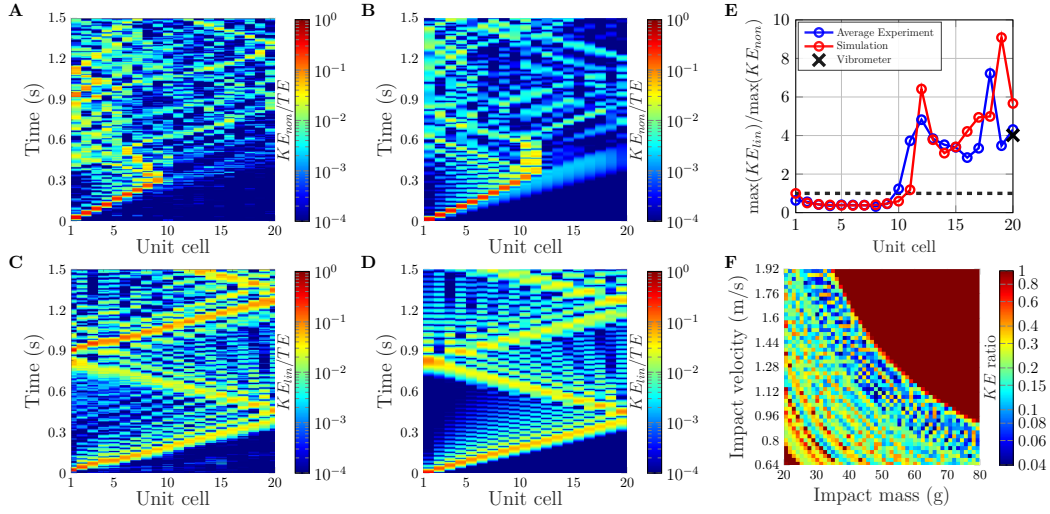


Figure 3.5. Experimental validation of the optimal nonlinear and linear chains, compared with simulation. A-D) Spatiotemporal evolution of kinetic energy in the system (normalized by the input kinetic energy, or initial total energy). The nonlinear chain is shown in A (experiment, nonlinear trial 1) and B (simulation), while the linear case is shown in C (experiment, linear trial 1) and D (simulation). The experimental spatiotemporal plots include a smoothing of displacement values to assist with noise induced by differentiating the discrete time camera data. The spatiotemporal plots for other trials are included in Supplementary Information Note 7. E) A ratio of maximum kinetic energy (linear/nonlinear) seen at each unit cell for both experiment and simulation. A value greater than 1 indicates superior performance of the nonlinear chain as compared to the linear. The experiment values are the average taken from three experimental trials. The X marks the average experimental value recorded by the vibrometer (see Supplementary Information Note 7 for the full data sets), which collected data from only the last unit cell. F) The simulated sensitivity of the KE ratio (truncated at 1) to impact conditions, wherein the simulation was run with the coefficients that were found experimentally from the nonlinear spring in Fig. 3.4D (that is, the physically achieved coefficients).

We note that the ratio shown in Fig. 3.5E is the inverse of KE ratio, for ease of visualization, such that larger numbers denote better impact protection. We see a larger discrepancy at the last two particles (Fig. 3.5E), which we attribute to non-ideal boundary conditions. We note that damping characterization (see Methods section) suggest the damping in both chains is similar (ζ of 0.005 for nonlinear and 0.003 for linear). Further, we show in Supplementary Information Note 6, that were the linear chain to have higher damping, *e.g.*, $\zeta = 0.006$, this would have negligible effect on the KE ratio. This highlights the value of nonlinear wave manipulation, where superior performance can be seen without heavy reliance upon damping.

A point of particular note, is that although the targeted conditions show excellent predicted performance, the behavior can be sensitive to small variations in impactor mass and velocity, as seen in the simulation data of Fig. 3.5F. The variability of the mass-velocity space is immediately apparent, with several very small regions of excellent performance (low KE ratios) surrounded by oscillating regions of lower performance (relatively higher KE ratios), and even several points of poor performance (KE ratio > 1). The optimum performance region targeted in this work sought out a region with relatively low drops in performance (relative to other regions explored via simulation), but nonetheless there still exist oscillatory performance impact conditions nearby. In order to more quantitatively describe this sensitivity, in Supplementary Information Note 4, we calculate the gradient of Fig. 3.5F, which shows $|\partial(\log_{10}(KE_{\text{ratio}}))/\partial M|$ can reach near 1 g^{-1} and $|\partial(\log_{10}(KE_{\text{ratio}}))/\partial V|$ can reach up to 40 s/m . This means that, for the most sensitive regions of the impact conditions landscape, a change in 1 g of impactor mass can result in an up to $\sim 6.7\times$ change in KE ratio, or a 0.01 m/s change in impactor velocity can result in an up to $\sim 2.5\times$ change in KE ratio. However, as with the case of the sensitivity to the nonlinear stiffness parameters, near our chosen optimum, the sensitivity is significantly lower, with $\partial(\log_{10}(KE_{\text{ratio}}))/\partial M = 0.16 \text{ g}^{-1}$ and $\partial(\log_{10}(KE_{\text{ratio}}))/\partial V = -7.8 \text{ s/m}$. This sensitivity is amplified due to the presence of bistability, in which the snapping (or lack thereof) of a single unit cell can push the system from one qualitative behavior well to another (see Supplementary Information Notes 4 and 9 for more in depth analysis and an example, respectively). The impactor velocities seen herein were not precise (ranging from 1.36 – 1.41 m/s, see Supplementary Information Note 7), and this, coupled with the aforementioned sensitivity provides an insight into variations in chain performance—namely, that the slight variations in impactor velocity we see in experiment have the potential to easily knock the system out of its optimal performance region, into one in which poorer performance is to be expected. This phenomenon reveals important characteristics regarding the sensitivity of the system, and more generally nonlinear dynamical systems wherein bifurcation can cause sharp changes in behavior [186]. We believe the proximity of regions of poor performance to regions of good performance (*e.g.*, Fig. 3.5F)

motivates a consideration of nearby conditions in future work. For instance, we expect there are application scenarios in which a region of reduced sensitivity to changes in stimuli may be desirable at the expense of slightly lowered performance. Despite the sensitivity of the system, however, per Fig. 3.5E the kinetic energy ratio (KE_{lin}/KE_{non}) remains greater than 1 (superior performance of the nonlinear chain compared to the linear) for both simulation and experiment once a critical number of unit cells has passed (unit cell 11 for the simulation, unit cell 10 in experiment).

3.3 Discussion

In this work, we have demonstrated a bilevel inverse design methodology for nonlinear wave tailoring in a mechanical system. Including the possibility of more highly discretized materials (*e.g.*, 100 unit cells, see Supplementary Information Note 5), our optimizations of nonlinear constitutive laws suggest the potential for over two orders of magnitude improvement (reduction) in kinetic energy transmission via the use of a nonlinear material compared to a comparative linear material. Our initial experiments on materials with fewer unit cells (20) show close agreement with our simulations, validating our bilevel design approach. We also observed large sensitivity of the kinetic energy transmission metric to small changes in nonlinearity and impact conditions, which we suggest highlights the need for high precision, free-form nonlinearity tailoring, as well as future study of nonlinear dynamical design for robustness-of-response to the presence of defects, disorder, and stimuli variation. Within the considered topic of impact mitigation, a near term question of future interest would be how such optimal nonlinearities would change for a different metric such as maximum transmitted force or peak tensile stress anywhere in the material. Similarly, although our proof of concept study focused on impact, we envision a wide range of applications that could make use of precisely tailored nonlinear signal transformation such as mechanical computing, acoustic signal, and image processing, vibration mitigation, and materials that autonomously respond and conduct directed work via

rapid shape-change. Additional future research areas include extension of this method to less scale separated dynamical (no lumped masses), higher-dimensional, irreversible constitutive, heterogeneous material, active, and coupled-physics settings.

3.4 Methods

DEM Simulations

We numerically integrate nondimensional Eq. (S8) in Supplementary Information Note 2 using a Runge-Kutta algorithm (ode45 in MATLAB) with impactor velocity V/V_0 and mass M/m applied to the impactor particle. The output and maximum integration timestep is selected by estimating the highest nondimensional frequency $f_{max} = \frac{1}{2\pi} \sqrt{\frac{k_{max}}{M_0}}$, where $k_{max} = \max(1, 1 + 2c_2 + 3c_3)$, such that the timestep $\Delta t = 1/(1000f_{max})$. The nondimensional displacement and velocity tolerances are set to 10^{-10} . The total energy conservation is checked for an undamped DEM system, and deviation is less than 0.1% over the entire simulation duration.

Structural Optimization

We include here further details about the shape optimization of the spring geometry, while noting that a full description of the method can be found in our previous work [177]. A level-set method is used to perform a nonlinear, displacement control, 2D continuum shape optimization. The spring is modeled using a 2D plane stress condition, with a Kirchhoff material model (linear elastic material model, with geometric nonlinearity included), as we have found this material model to be a good representation of polycarbonate throughout displacement ranges which do not reach the plasticity threshold of the material. The optimization performed herein was solved with a uniform mesh consisting of 750×750 quadrilateral elements. A symmetry boundary condition (rollers) is applied along the bottom edge of the optimization domain, such that only one half of the spring need be simulated. The top edge of the domain has a fixed boundary condition enforced. A 1D applied displacement is applied at the bottom right edge of

the domain, where the connector to the adjacent spring would exist in the physical system. These conditions, along with the initial condition supplied to the optimizer, are illustrated in Note 6 in the Supplementary Information.

Prior to manufacture and experimental tests, the force displacement output from the optimization process was further confirmed via a FEM simulation in COMSOL Multiphysics. Following the verification process outlined in our previous work [177], the optimal level set was converted to a 2D geometry in COMSOL, and a quasi-static simulation was performed. This simulation similarly used 2D plane stress, with a Kirchhoff material model and the same applied boundary conditions as the optimization process. The COSMOL simulation, however, employed a body-fitted mesh consisting of 20,447 triangular elements. The results, shown in Fig. 3.4D, confirm the accuracy of the optimization simulation.

As outlined in Eq. 3.2, the objective function for the optimization is taken to be the ratio of polynomial coefficients resulting from the force-displacement curve of the current design. This polynomial is fit to the force-displacement curve using the equation $c = V^{-1}C$, in which V is the Vandermonde matrix, and C is compliance (we note that herein, we use lowercase c to refer to polynomial coefficients, and uppercase C to refer to compliance). Fitting to compliance, rather than force, is done for ease of sensitivity calculation, as compliance optimization is a well known optimization problem. Noting that $C = F\Delta x$ (in which Δx is displacement), it is a simple matter to transition between force and compliance. We can then write the sensitivity for the polynomial ratio objective as a combination of known compliance sensitivity terms and sensitivity terms related to the fitting of the polynomial.

$$\frac{\partial c_i}{\partial \Omega} = \sum_{j=1}^m \frac{\partial c_i}{\partial C_j} \frac{\partial C_j}{\partial \Omega} = \sum_{j=1}^m V^{-1}(i, j) \frac{\partial C_j}{\partial \Omega}, \quad (3.3)$$

where Ω refers to the level set domain, i refers to the degree of polynomial, j refers to the displacement step, and m is the total number of displacement points under consideration (see our previous work for more details[177]).

Unit Cell Design and Manufacturing

After the nonlinear spring had been designed via optimization, the design was resized to the experiment scale (wherein the length of one spring, a_s , was taken to be 59 mm). The single spring design was reflected over the symmetry condition, and in order to minimize the non-longitudinal motion of the masses, a second set of nonlinear springs was added in parallel to the first. A single unit cell (shown in Fig. 3.4C) was fabricated by cutting the shape out of a polycarbonate sheet via computer-numerical-control (CNC) milling. This milled shape was then sanded down at the edges to fit smoothly into a rectangular stainless steel frame, which was commercially manufactured via sheet cutting, and secured in-plane with an acrylic backing bolted into the frame and glued to the milled spring (see Note 7 in the Supplementary Information for a visualization). We note the design of the frame surrounding a spring is particularly important in properly imposing boundary conditions, and thus critical in matching simulation predicted force displacement curves. The choice of a stainless steel frame herein was made in order to meet these criteria, while still allowing for the milling of the spring to fit within the manufacturing constraints of the manufacturing equipment.

A single unit cell was tested quasi-statically to confirm the performance of the spring, as shown in Fig. 3.4D. Repeated, cyclic quasi-static loading tests were also performed to confirm that no onset of plasticity or fatigue occurs during the dynamic experiment (see Supplementary Information Note 6).

Data Collection

The motion of each unit cell was captured with the use of cameras mounted above the chain. The length of the chain necessitated the use of multiple cameras to capture the motion all unit cells. Each experimental trial therefore has four videos associated with it, shot in slow motion at 240 fps on four iPhones, with each video overlapping by at least one unit cell to ensure proper spatial synchronization and the capture of all motion. For each trial, the cameras and unit

cells were spaced such that camera 1 captured unit cells 1-6, camera 2 captured unit cells 4-11, camera 3 captured unit cells 9-16, and camera 4 captured unit cells 14-20. Video processing was performed in MATLAB. Temporal synchronization between each video was achieved by a visual signal which caused a fluctuation in intensity of light, which could then be detected in each video and used to synchronize the times between the recording devices. Tracking of each particle was achieved with the use of colored markers on each unit cell. Post processing in MATLAB allowed each frame to be separated into discrete color channels, allowing for the isolation and tracking of red, blue, and green markers (blue was used for the impactor, green for the back edge of each unit cell, and an additional red marker for unit cells which were covered by overlapping camera fields of view, in order to enable spatial synchronization of the data from each camera).

Damping Characterization

In order to characterize the damping ratio ζ of the manufactured springs, the power spectrum was experimentally measured, generated from a low-amplitude 1 ms duration square pulse excitation applied to a single spring via electrodynamic shaker. A Lorentzian function was numerically fit to the response for both the nonlinear and linear spring cases. The experimental setup for both cases are shown in Supplementary Information Note 6, where the single unit cell was hung horizontally using fishing lines, and the end of the connector, which was connected to the center of the spring via bolts and nuts, was clamped to impose a fixed boundary condition (FBC). The pulse excitation was provided by a function generator (FG, Tektronix AFG3022C), controlled through MATLAB, and applied via an electrodynamic shaker (The Modal Shop K2007E01) equipped with a stinger, whose tip was manually set at a small distance (within 1 mm) away from the side surface of the unit cell. A laser Doppler vibrometer (LDV, Polytec PSV 400) was used to record the dynamical response of the unit cell in velocities. Data was collected by measuring the side surface of the unit cell (averaged three times for each test), where the LDV and the FG were synchronized through a common trigger signal for repeatability of the averaging process. Measured dynamical responses, which were processed to account for

the tilted angle between the LDV scanning head and the unit cell, are shown in Supplementary Information Note 6. The normalized power spectrum was obtained by taking the square of the Fourier transform (FFT) of time domain data and then normalizing its maximum value. The FFT was taken using the built-in *fft* command in MATLAB. The normalized $|\text{FFT}|^2$ result was fit to a Lorentzian function of the following form

$$L(f) = \frac{A}{\pi} \frac{\Gamma/2}{(f - f_0)^2 + (\Gamma/2)^2}, \quad (3.4)$$

where A is the amplitude parameter, f_0 is the central frequency, and Γ is the full width at half maximum in frequency. The fitting process was done by using the built-in *fit* command in MATLAB. The Q factor was found by taking f_0/Γ from the numerical fitting, which are approximately 92 for the nonlinear and 177 for the linear spring unit cell. Based on these Q factors, by using the equation $\zeta = 1/(2Q)$, we calculated the damping ratios ζ as 0.005 and 0.003 for nonlinear and linear chains, respectively, which were used in the numerical simulations.

3.5 Supplemental Information

Note 1: Two and three dimensional nonlinear mesostructured material analogs

In Fig. 3.6, we show the concepts for two- and three-dimensional (2D and 3D) generalization of the optimized nonlinear mesostructured material described in the main text. We note that relative transverse and rotation between the masses, in addition the longitudinal translation described in the main text, would need to be accounted for in any design optimized for such higher dimensions (which has not been considered in this work).

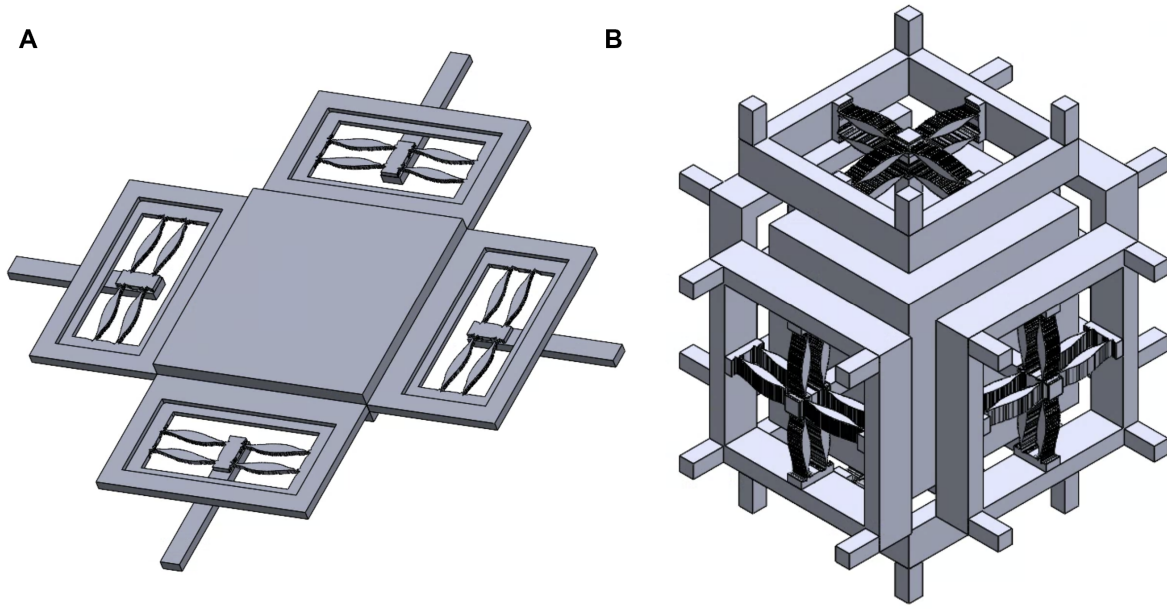


Figure 3.6. A) 2D generalization of an optimized nonlinear mesostructured material. B) 3D generalization of an optimized nonlinear mesostructured material.

Note 2: Reduced order discrete element model and non-dimensionalization

Our reduced order discrete element model (DEM) of a nonlinear material (Fig. 3.7) includes N layers of unit cells. Each unit cell consists of a lumped mass m , a massless spring $f^*(\Delta x^*)$ where Δx^* is the spring stretch such that Δx^* and f^* are positive in tension, and a linear inter-site viscous damper η^* . The equation of motion of the i th unit cell can be written as

$$m\ddot{x}_i^* + f^*(x_i^* - x_{i-1}^*) - f^*(x_{i+1}^* - x_i^*) + \eta^*(-\dot{x}_{i+1}^* + 2\dot{x}_i^* - \dot{x}_{i-1}^*) = 0, \quad (3.5)$$

where x_i^* is the displacement of the i th particle from its rest position.

In this work, we consider cubic polynomial nonlinear springs in compression and linear springs in tension. Considering first then the compressional behavior, e.g., $x_{i+1}^* \leq x_i^*$ and

$x_i^* \leq x_{i-1}^*$, Eq. (3.5) can be replaced by

$$\begin{aligned} m\dot{x}_i^* - c_1^*(x_{i+1}^* - x_i^*) + c_2^*(x_{i+1}^* - x_i^*)^2 - c_3^*(x_{i+1}^* - x_i^*)^3 \\ + c_1^*(x_i^* - x_{i-1}^*) - c_2^*(x_i^* - x_{i-1}^*)^2 + c_3^*(x_i^* - x_{i-1}^*)^3 + \eta^*(-\dot{x}_{i+1}^* + 2\dot{x}_i^* - \dot{x}_{i-1}^*) = 0. \end{aligned} \quad (3.6)$$

We note that the coefficient c_2^* is opposite sign from c_1^* and c_3^* , which we choose for convenience.

The overdot on the variables with the $*$ denotes the time derivative, such that $\dot{x}^* = dx^*/dt^*$.

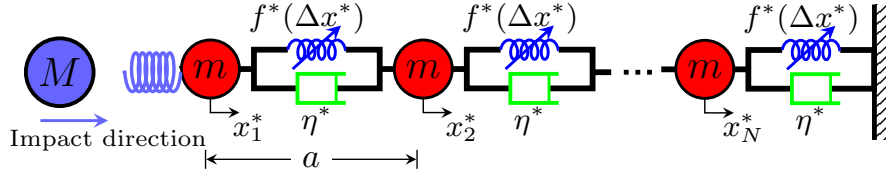


Figure 3.7. Schematic of the DEM. Horizontal arrows on the masses denote positive x^* .

Next, all variables and parameters are normalized by the length of a unit cell, a , the mass of a unit cell, m , and/or the linear stiffness of the spring, c_1^* , as follows

$$\begin{aligned} x_i = \frac{x_i^*}{a}, \quad t = \frac{t^*}{\sqrt{m/c_1^*}}, \quad \frac{dx_i}{dt} = \frac{\sqrt{m/c_1^*}}{a} \frac{dx_i^*}{dt^*}, \quad \frac{d^2x_i}{dt^2} = \frac{m}{c_1^* a} \frac{d^2x_i^*}{dt^{*2}}, \\ c_2 = \frac{c_2^* a}{c_1^*}, \quad c_3 = \frac{c_3^* a^2}{c_1^*}, \quad \zeta = \frac{\eta^*}{2\sqrt{mc_1^*}}, \end{aligned} \quad (3.7)$$

and the linear sound speed is $V_0 = a\sqrt{c_1^*/m}$.

The nondimensional equation of motion of the i th unit cell is then given by

$$\begin{aligned} \ddot{x}_i - (x_{i+1} - x_i) + c_2(x_{i+1} - x_i)^2 - c_3(x_{i+1} - x_i)^3 \\ + (x_i - x_{i-1}) - c_2(x_i - x_{i-1})^2 + c_3(x_i - x_{i-1})^3 + 2\zeta(-\dot{x}_{i+1} + 2\dot{x}_i - \dot{x}_{i-1}) = 0. \end{aligned} \quad (3.8)$$

The overdot on variables without the $*$ denotes the derivative with respect to non-dimensional time, such that $\dot{x} = dx/dt$.

The impactor, with mass of M and initial velocity of V , is assumed to interact with the

nonlinear material via a contact spring. A contact spring featuring nonlinear stiffness, positioned between the first unit cell and the impactor mass, has been incorporated into the model to allow smooth contact and free release upon rebound. The contact spring is a Hertzian-like [187] nonlinear contact spring of the form

$$F_H^*(x_0^*, x_1^*) = C_{imp} [x_0^* - x_1^*]_+^{3/2}, \quad (3.9)$$

where the $[\cdot]_+$ denotes that the quantity in between the brackets only takes positive values and equals zero when negative, and F_H^* is positive when in compression. The provision of compressed force between the impactor mass and the material through bouncing force occurs only if $x_0^* > x_1^*$. The non-dimensional contact force is

$$F_H(x_0, x_1) = \frac{F_H^*(x_0^*, x_1^*)}{c_1^* a} \quad (3.10)$$

such that

$$F_H(x_0, x_1) = \frac{C_{imp} \sqrt{a}}{c_1^*} [x_0 - x_1]_+^{3/2}. \quad (3.11)$$

The entire nondimensional DEM of the impact dynamics system consisting of an N -

layered nonlinear metamaterial is thus

$$\left\{ \begin{array}{l} m_{im}\ddot{x}_0 + F_H(x_0, x_1) = 0 \quad (x_0 > x_1) \\ \ddot{x}_i - (x_{i+1} - x_i) + c_2(x_{i+1} - x_i)^2 - c_3(x_{i+1} - x_i)^3 \\ + 2\zeta(-\dot{x}_{i+1} + \dot{x}_i) - F_H(x_0, x_1) = 0 \quad (i = 1) \\ \ddot{x}_i - (x_{i+1} - x_i) + c_2(x_{i+1} - x_i)^2 - c_3(x_{i+1} - x_i)^3 \\ + (x_i - x_{i-1}) - c_2(x_i - x_{i-1})^2 + c_3(x_i - x_{i-1})^3 \\ + 2\zeta(-\dot{x}_{i+1} + 2\dot{x}_i - \dot{x}_{i-1}) = 0 \quad (2 \leq i \leq N-1) \\ \ddot{x}_i + x_i - c_2x_i^2 + c_3x_i^3 + (x_i - x_{i-1}) + c_2(x_i - x_{i-1})^2 + c_3(x_i - x_{i-1})^3 \\ + 2\zeta(2\dot{x}_i - \dot{x}_{i-1}) = 0 \quad (i = N), \end{array} \right. \quad (3.12)$$

where $m_{im} = M/m$, and Eq. (3.12) is valid when the springs are in compression. When the springs are in tension, we set $c_2 = 0$ and $c_3 = 0$.

Note 3: Characteristics of the nonlinear spring (3rd order polynomial)

The non-dimensional nonlinear spring in this study is chosen to conform to a third-order polynomial representation, expressed as $f(\Delta x) = f^*(\Delta x^*)/c_1^*a = \Delta x + c_2(\Delta x)^2 + c_3(\Delta x)^3$. In this section, we describe $\Delta x \in [0, 1]$ for simplicity, despite compression being considered in the main text. For compression ($\Delta x < 0$) the only thing that changes from the analysis is that the sign of c_2 is flipped for $\Delta x < 0$. We also set $c_3 > 0$ for simplicity. By manipulating both the sign and magnitude of c_2 , the function $f(\Delta x)$ exhibits the potential for either two extrema (a local maximum and a local minimum), a single extremum (local maximum), or none at all (Fig. 3.8). We consider each case further in the following.

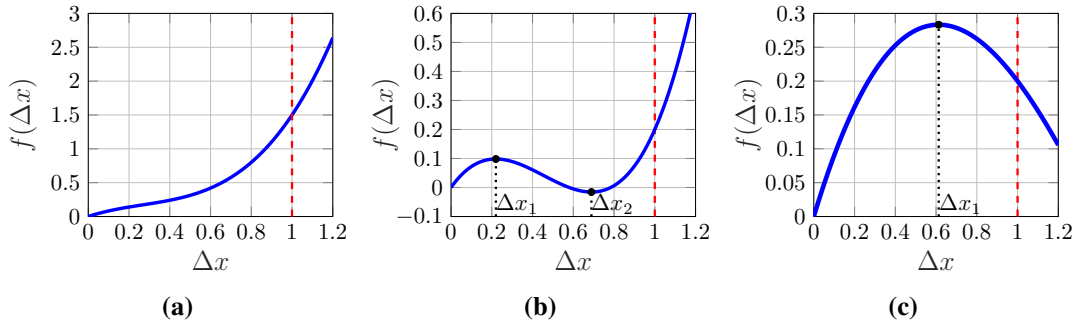


Figure 3.8. Force-displacement characteristics of third-order polynomial nonlinear springs that exhibit the following behaviors: (a) monotonic increment, (b) bistability/snap-through, and (c) local maximum in the function $f(\Delta x)$.

3.1 Monotonic increase of $f(\Delta x)$

For monotonic increase, we must satisfy the condition

$$f'(\Delta x) \geq 0, \quad (3.13)$$

where $f' = df/d\Delta x$, such that

$$1 + 2c_2\Delta x + 3c_3(\Delta x)^2 \geq 0. \quad (3.14)$$

For our considered range of parameters, Eq. (3.14) is always satisfied if

$$c_2 > -\sqrt{3c_3}, \quad (3.15)$$

which corresponds to the cases of no real roots or $c_2 \geq 0$.

An additional condition for ensuring a monotonic increase in the function $f(\Delta x)$ for $\Delta x \in [0, 1]$ is that the local maximum of $f(\Delta x)$ should be situated at $\Delta x \geq 1$. In such a case, the small-valued root Δx_1 of $f'(\Delta x) = 0$ must satisfy

$$\Delta x_1 \geq 1 \quad (3.16)$$

where

$$\Delta x_1 = \frac{-c_2 - \sqrt{c_2^2 - 3c_3}}{3c_3}. \quad (3.17)$$

For real Δx_1 (Eq. (3.17)), the coefficients must thus satisfy

$$c_2 \leq -\sqrt{3c_3} \quad (3.18)$$

and

$$-\sqrt{c_2^2 - 3c_3} \geq c_2 + 3c_3. \quad (3.19)$$

From Eq. (3.19), we obtain the criteria

$$c_2 \leq -3c_3 \quad (3.20)$$

and

$$c_2 \geq -\frac{1+3c_3}{2}. \quad (3.21)$$

Considering Eqs. (3.15), (3.18), (3.20) and (3.21), we can then say that $f(\Delta x)$ exhibits a monotonic increase when the coefficients satisfy: i) $c_2 > -\sqrt{3c_3}$; or ii) $c_2 \leq -\sqrt{3c_3}$, $c_2 \leq -3c_3$, and $c_2 \geq -(1+3c_3)/2$ simultaneously.

3.2 Bistability or snap-through of $f(\Delta x)$

To establish a bistable curve, inclusive of snap-through behavior, it is necessary that the local maxima and minima both occur within the interval of $\Delta x \in (0, 1)$. The strain (or potential) energy must also remain positive in this same interval. To satisfy the first criterion, the roots of $f'(\Delta x) = 0$

$$\Delta x_{1,2} = \frac{-c_2 \pm \sqrt{c_2^2 - 3c_3}}{3c_3} \quad (3.22)$$

must satisfy

$$0 < \Delta x_{1,2} < 1. \quad (3.23)$$

As before, to obtain real roots

$$c_2 \leq -\sqrt{3c_3} \quad (3.24)$$

must be satisfied. As $\sqrt{c_2^2 - 3c_3} \geq 0$, Eq. (3.23) can be rewritten as

$$-c_2 - \sqrt{c_2^2 - 3c_3} > 0, \quad (3.25)$$

and

$$-c_2 + \sqrt{c_2^2 - 3c_3} < 3c_3. \quad (3.26)$$

Equation (3.25) is always satisfied for $c_2 \leq -\sqrt{3c_3}$. Equation (3.26) generates the two conditions

$$c_2 > -3c_3, \quad (3.27)$$

and

$$c_2 > -(1 + 3c_3)/2. \quad (3.28)$$

Next, to satisfy the condition of potential energy $P(\Delta x) > 0$ we define

$$P(\Delta x) = \int_0^1 f(\Delta x) d\Delta x \quad (3.29)$$

which gives the condition

$$\frac{1}{2} + \frac{c_2}{3} + \frac{c_3}{4} > 0 \quad (3.30)$$

that simplifies to

$$c_2 > -\frac{3}{2} - \frac{3c_3}{4}. \quad (3.31)$$

Combining Eqs. (3.24), (3.27), (3.28), and (3.31), when the coefficients satisfy $c_2 > \max[-(1 + 3c_3)/2, -3c_3, -3/2 - 3c_3/4]$, and $c_2 \leq -\sqrt{3c_3}$, the function $f(\Delta x)$ can exhibit bistability/snap-through.

3.3 Local maximum of $f(\Delta x)$ for $\Delta x \in (0, 1)$

When the function only has a local maximum within $\Delta x \in (0, 1)$ and no local minimum, we should ensure $0 < \Delta x_1 < 1$ and $\Delta x_2 > 1$, such that

$$0 < \frac{-c_2 - \sqrt{c_2^2 - 3c_3}}{3c_3} < 1, \quad (3.32)$$

and

$$\frac{-c_2 + \sqrt{c_2^2 - 3c_3}}{3c_3} > 1. \quad (3.33)$$

Equation (3.32) gives the conditions

$$c_2 \leq -\sqrt{3c_3}, \quad (3.34)$$

and

$$c_2 < -\frac{1+3c_3}{2}. \quad (3.35)$$

Equation (3.33) can be rewritten as

$$\sqrt{c_2^2 - 3c_3} > c_2 + 3c_3. \quad (3.36)$$

If $c_2 + 3c_3 \leq 0$, Eq. (3.36) is always satisfied, and results in the condition

$$c_2 \leq -3c_3. \quad (3.37)$$

On the other hand, if $c_2 + 3c_3 > 0$, we must have

$$c_2 < -\frac{1+3c_3}{2} \quad (3.38)$$

to satisfy Eq. (3.36), which is equivalent to Eq. (3.35).

Considering Eqs. (3.34), (3.35), (3.37) and (3.31), the parameters thus need to satisfy

$$\begin{aligned} c_2 &> -\frac{3}{2} - \frac{3c_3}{4} \quad \text{and} \\ c_2 &< \min\left(-\frac{1+3c_3}{2}, -\sqrt{3c_3}, -3c_3\right), \end{aligned} \quad (3.39)$$

or

$$\begin{aligned} c_2 &> \max\left(-\frac{3}{2} - \frac{3c_3}{4}, -3c_3\right) \quad \text{and} \\ c_2 &< \min\left(-\frac{1+3c_3}{2}, -\sqrt{3c_3}\right). \end{aligned} \quad (3.40)$$

Equation (3.40), however, lacks a valid set. As a result, the occurrence of a single local maximum for $f(\Delta x)$ within $0 < \Delta x < 1$ is contingent upon satisfying Eq. (3.39).

Note 4: Sensitivity to system and impactor properties, and sharp performance changes upon unit cell snapping

In Fig. 3.9(a,b), we show the sensitivity of the $\log_{10}$ of the data in the inset of Fig. 2C in the main text (maximum KE experienced at the last particle normalized by initial energy of the impactor) with respect to the nonlinear coefficients c_2 and c_3 , respectively. Similarly, in Fig. 3.9(c,d), we show the sensitivity of the $\log_{10}$ of the data in the Fig. 5F in the main text (KE ratio) with respect to the impactor conditions M and V , respectively.

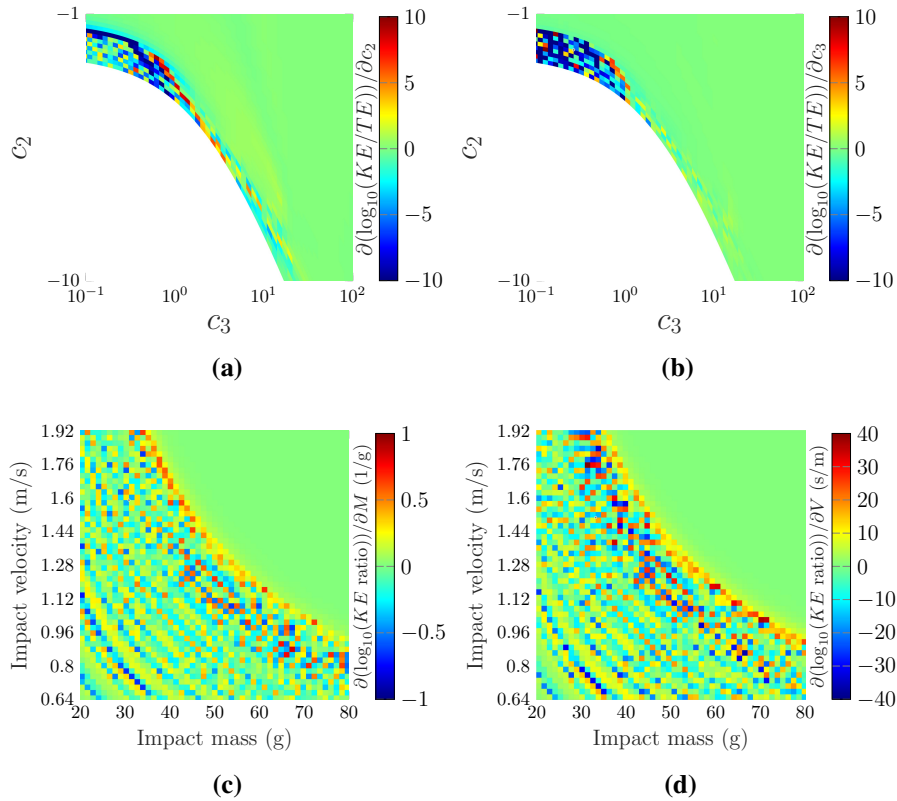


Figure 3.9. Performance gradients. Sensitivity of the $\log_{10}$ of the data in the inset of Fig. 3.2C in the main text (maximum KE experienced at the last particle normalized by initial energy of the impactor [TE]) with respect to the nonlinear coefficients (a) c_2 and (b) c_3 ($\partial(\log_{10}(KE/TE))/\partial c_2$ and $\partial(\log_{10}(KE/TE))/\partial c_3$, respectively). Sensitivity of the $\log_{10}$ of the data in Fig. 3.5F in the main text (KE ratio) with respect to the impactor conditions (c) M and (d) V ($\partial(\log_{10}(KE \text{ ratio}))/\partial M$ and $\partial(\log_{10}(KE \text{ ratio}))/\partial V$, respectively).

We next demonstrate the sharp changes in performance (maximum kinetic energy experi-

enced at the end of the linear chain, divided by the maximum kinetic energy experienced at the end of the nonlinear chain) when an additional unit cell in the chain snaps. Here we consider a slightly different, but still bistable, nonlinear spring from the main text. The parameters for this system are $f(\Delta x) = \Delta x + 87\Delta x^2 + 1778\Delta x^3$, where the linear stiffness is set as $c_1^* = 1.0454$ kN/m, the impactor mass $M_0 = 40$ g, and the length of a unit cell $a = 125$ mm. In Fig. 3.10, we see very large, periodic jumps in performance (a factor of greater than 10 times) as the impactor velocity is increased even by very small amounts of $\sim 3\%$ (~ 0.03 m/s). Here we consider a shorter simulation duration, just over the one-way transit time of a pulse through the material.

Several of the simulations underlying the parameter sweep of Fig. 3.10 can be seen in Fig. 3.11, for impactor velocities corresponding to several sequential maximum amplitude points in Fig. 3.10 ($V = \{1.354, 1.406, 1.454, 1.497\}$ m/s). It can be seen in Fig. 3.11, that each of these high amplitude points sequentially correspond to one later unit cell in the chain snapping and terminating the motion of the main initial pulse propagating through the system.

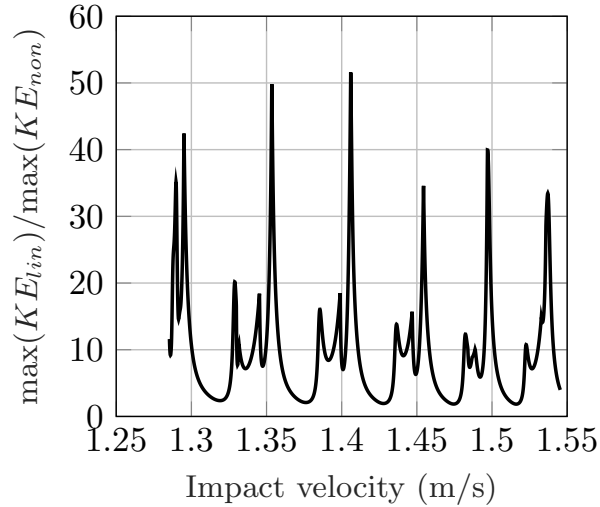


Figure 3.10. The maximum kinetic energy (linear/nonlinear) versus impactor velocity at the last unit cell using a new set of nonlinear spring coefficients. The new nonlinear mechanical response has a similar behavior to the one used in the experiment with the form of $f(\Delta x) = \Delta x + 87\Delta x^2 + 1778\Delta x^3$. The linear stiffness is set as $c_1^* = 1.0454$ kN/m, the impactor mass is 40 g, and the length of a unit cell is 125 mm.

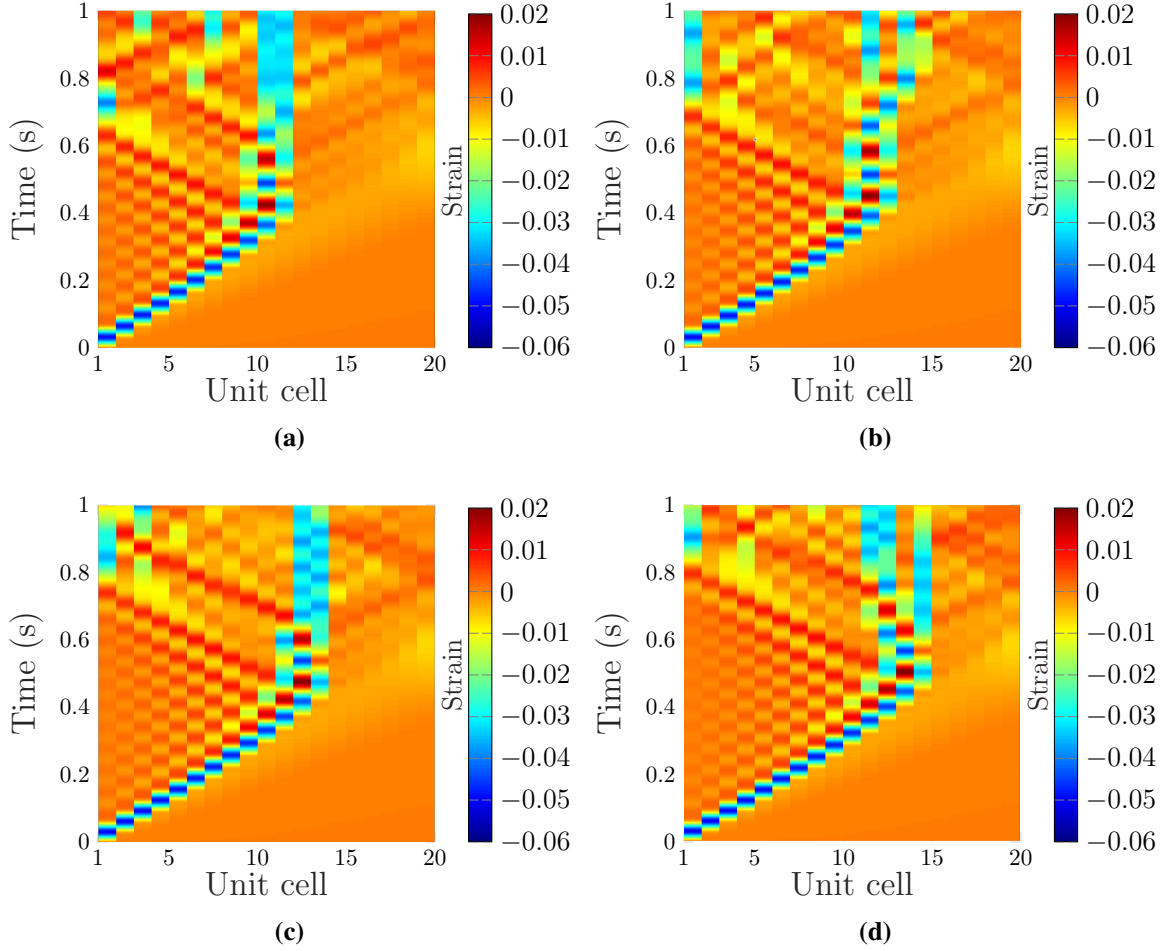


Figure 3.11. Spatiotemporal evolution of strain in the nonlinear chain for different impactor velocities corresponding to several of the highest amplitude KE ratio peaks in Fig. 3.10. (a) $V = 1.354$ m/s, (b) $V = 1.406$ m/s, (c) $V = 1.454$ m/s, and (d) $V = 1.497$ m/s.

Note 5: Additional DEM results

Figure 3.12 illustrates the best KE ratios at the end of the material and their corresponding nonlinear spring coefficients for varied impactor mass and velocities ($N = 20$, $\zeta = 0.025$). Figure 3.13 shows the best KE ratios at the mid-point of the material and the corresponding coefficients for a 100-unit-cell chain and $\zeta = 0.025$.

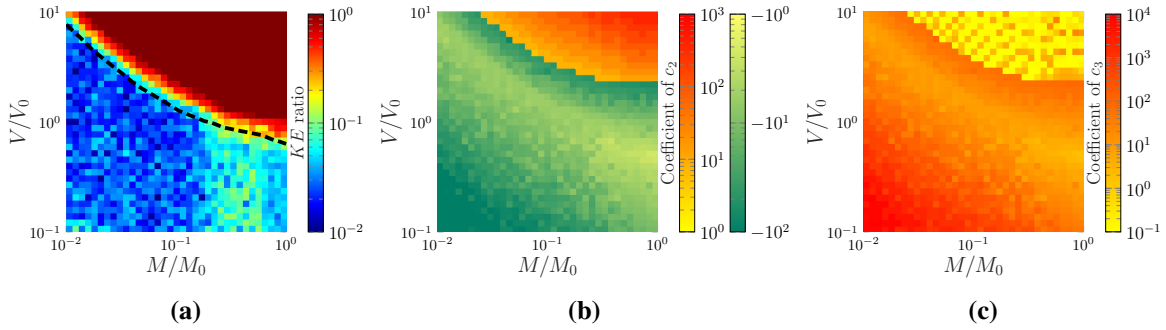


Figure 3.12. (a) KE ratio at the end of the material with respect to impactor mass and velocity and corresponding nonlinear spring coefficients (b) c_2 and (c) c_3 for a energy absorbing material with $N = 20$, $\zeta = 0.025$. The impactor mass and velocity are swept from $0.01M_0$ to M_0 , and $0.1V_0$ to $10V_0$, respectively.

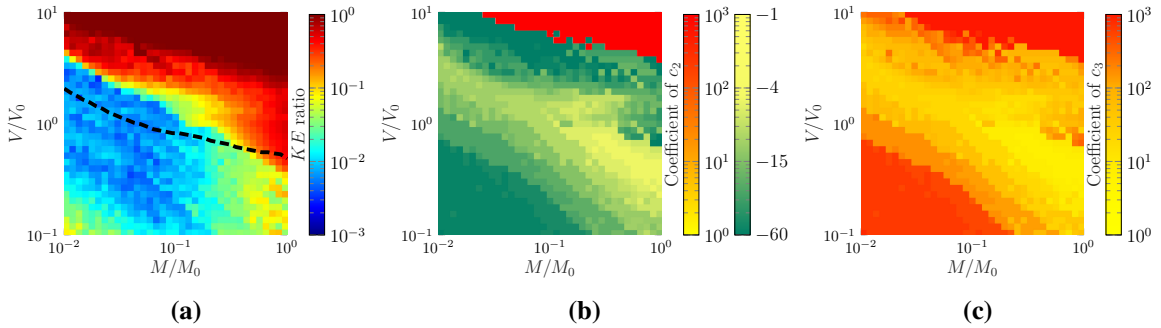


Figure 3.13. (a) KE ratio at the middle of the material as a function of impactor mass and velocity and corresponding nonlinear spring coefficients (b) c_2 and (c) c_3 for a energy absorbing material with $N = 100$, $\zeta = 0.025$. The impactor mass and velocity are swept from $0.01M_0$ to M_0 , and $0.1V_0$ to $10V_0$, respectively.

Note 6: Unit cell design and damping characterization

The initial condition used to optimized the unit cell mesostructure is depicted in Fig. 3.14. The boundary conditions imposed are also depicted — fixed along the top edge, rollers along the bottom edge (allowing for a symmetric reflection of the structure across the bottom edge for a two spring unit cell), with an applied displacement across the right edge, from 0 to 0.1 of the domain length (a region defined by $x = 1, y = 0$ to 0.1).

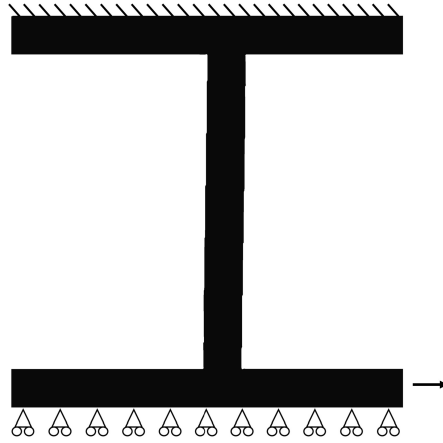


Figure 3.14. Initial condition for the topology optimization of the nonlinear spring.

The top edge fixed boundary is particularly important for the bistable design, as the transition from one stable state to another requires it to pass through a compressive deformation that presses against both the top and bottom edges. If the frame housing the optimized spring is not strong enough relative to the spring to impose a sufficiently rigid boundary, the bistability of the response is reduced. Accordingly, the frame (as shown in Fig. 4C in the main text) for each spring was designed to be higher modulus and thicker than the spring itself, such that boundary conditions would be sufficiently rigid to enable the nonlinear response. This was confirmed via FEM simulation prior to manufacture, and via quasi-static experiment (see Fig. 3.4D in the main text) once the design had been manufactured.

The spring used for the linear chain is shown in Fig. 3.15. The final manufactured design is shown on the left panel of the figure. We note that four individual linear springs were used in

the final design. More springs were added to increase the stiffness of the linear design such that it would be closer to that of the nonlinear design. The final experimental linear stiffness of the nonlinear spring was found to be 1.0598 kN/m, while the linear spring was found to be 1.0454 kN/m, both as measured from quasi-static tests. The green marker used to track unit cell motion is visible on the right edge of the manufactured unit cell. The quasi-static test of the linear spring can be seen in Fig. 3.16.

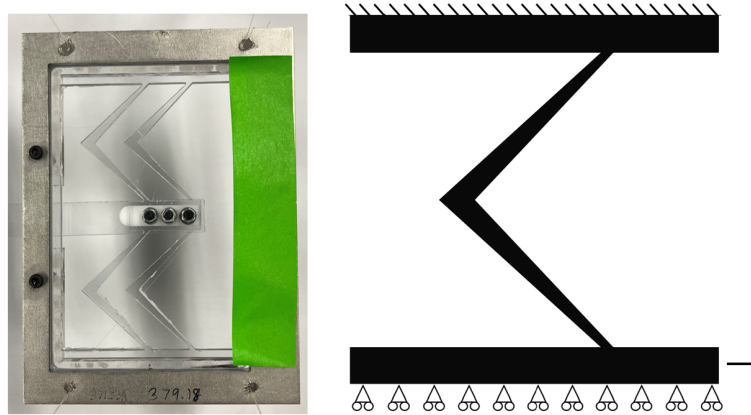


Figure 3.15. Design of the linear spring used as the control for comparison with the optimized nonlinear spring. The right panel shows the design of a single linear spring, including the boundary conditions. The left panel shows the final manufactured linear spring unit cell, along with the green marker used for image tracking in the experiment videos on the right edge.

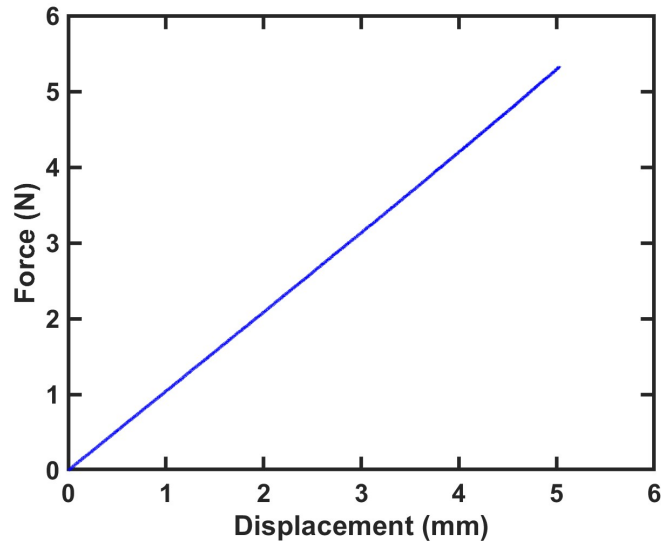


Figure 3.16. Quasi-static experimental test of the manufactured linear spring, confirming stiffness and linearity of behavior.

As mentioned in the main text, there was some concern about the onset of plasticity and the effects on the optimized structure of repeated loading due to multiple experimental trials. Multiple cycles of quasi-static loading tests were therefore conducted to confirm that the response of the structure did not appreciably degrade over multiple loading cycles. The results of this testing are shown in Fig. 3.17. Five tests were conducted to just over half the maximum designed range of displacement (4 mm), and five were conducted up to 7 mm. We note that the spring was pressed slightly down while fixing it into the load frame, and is therefore not necessarily beginning from the precise equilibrium state in these tests, but this should have no bearing on the intended purpose (which was to confirm no onset of plasticity).

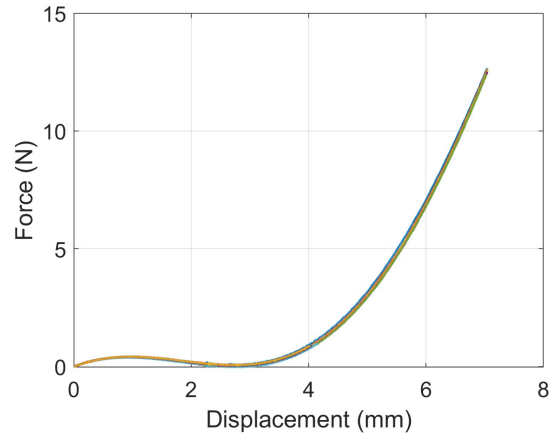


Figure 3.17. Results of quasi-static cyclic loading testing. A total of 10 tests were run, with tests 1 through 5 being run to a maximum displacement partially through the expected displacement range, and tests 6 through 10 sweeping through the entire expected operating displacement range of the structure.

The plots associated with the damping characterization, described in the main text in the Methods section, are included here. Fig. 3.18(a) and (b) show the experimental setup. Measured dynamical responses, which were processed to account for the tilted angle between the LDV scanning head and the unit cell, are shown in Fig. 3.19(a) and (c). The normalized power spectrum is shown in Fig. 3.19(b) and (d).

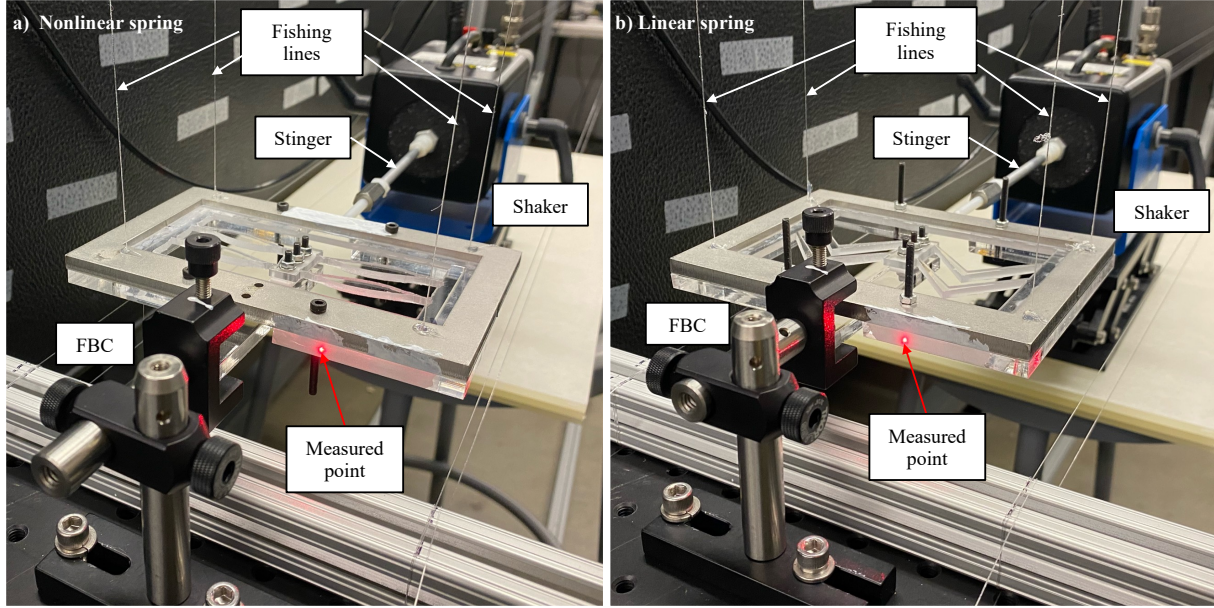


Figure 3.18. Experimental setup for characterizing the damping ratio of a single unit cell for (a) nonlinear and (b) linear chains. LDV (not appear in the photos) was placed behind the metal clamp that serves as a fixed boundary condition (FBC). The tilted angle of the LDV has been considered and processed in the data analysis.

In Fig. 3.20, we show the simulated effect of differences in damping on KE ratio. The two damping values considered are the experimentally characterized damping ratio for the linear chain ($\zeta = 0.003$) compared to a damping ratio for the linear chain of just larger than that measured for the nonlinear chain ($\zeta = 0.006$). This level of difference in damping can be seen to have minimal effect on the performance metric, confirming the dominant effect of varied nonlinearity.

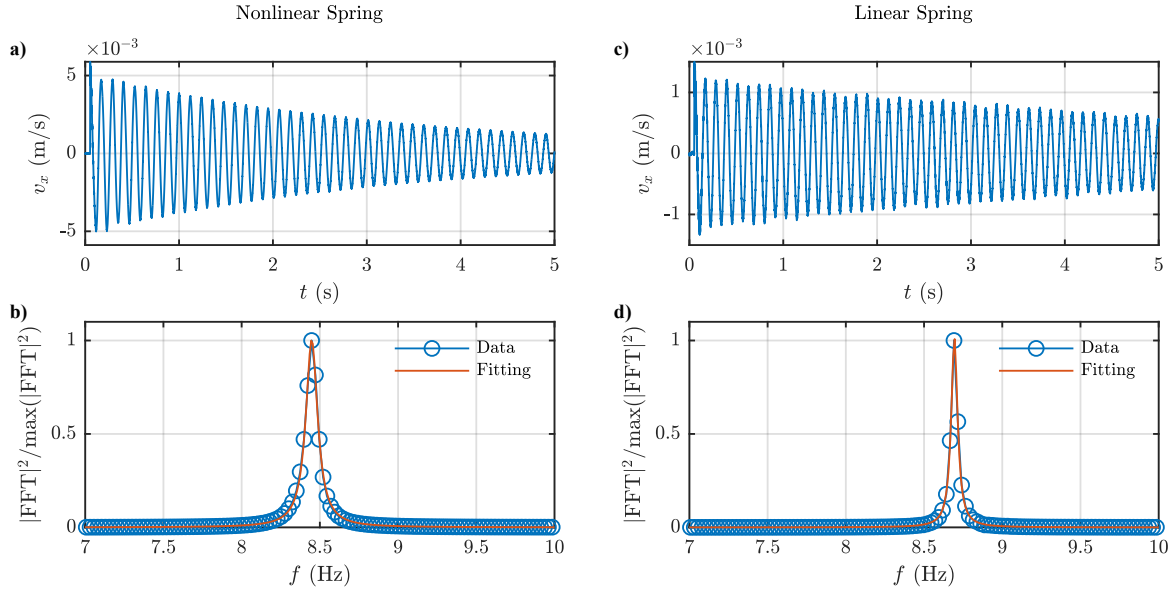


Figure 3.19. Experimental results for characterizing the damping ratio of a single unit cell for (a-b) nonlinear and (c-d) linear chains. (a,c) Processed time domain data (first 5 s), where the pulse excitation was applied at 20 ms. (b,d) Normalized power spectrum of the entire time domain data (about 41 s) with the fitting line of the Lorentzian function.

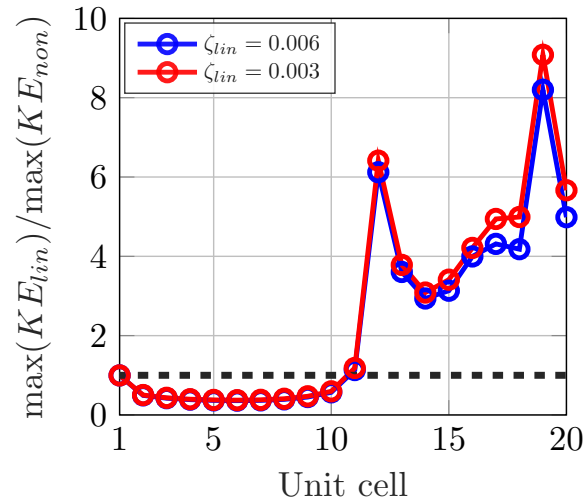


Figure 3.20. The maximum kinetic energy (linear/nonlinear) seen at each unit cell for simulation with different linear damping ratios. The nonlinear spring is fixed with $\zeta = 0.005$, and the linear spring has damping ratios of $\zeta_{lin} = 0.006$ and $\zeta_{lin} = 0.003$.

Note 7: Additional experimental details and results

A more thorough view of the experimental setup, comparing the experimental system to the DEM, is presented in Fig. 3.21. Further details of the unit cell and connectors are shown in Figure 3.22.

The 24 videos associated with the experiments (4 each for 3 nonlinear experiments and 3 linear experiments) are included in the following data repository: Boechler, Nicholas (2024), “Customizable wave tailoring materials enabled by nonlinear bilevel inverse design 1”, Mendeley Data, V1, doi: 10.17632/2wgwfy2wfg.1. Table 3.1 outlines the naming scheme, as well as the specific impactor velocity values measured by the cameras for each trial. In addition to the tracked unit cell location collected by the cameras, a vibrometer (specifically, a Polytec PSV 400 laser vibrometer) was pointed at the last unit cell of each chain (unit cell 20), in order to have a second measurement of the velocity of the last unit cell.

Table 3.1. List of experimentally captured video files and test details (corresponding to data shown in the main text).

Video Name (1-4 for each test)	Spring Tested	Trial Number	Impactor Velocity (m/s)
Main_NonlinTrial1_Vid1.mov through _Vid4.mov	Updated Nonlinear	1	1.38
Main_NonlinTrial2_Vid1.mov through _Vid4.mov	Updated Nonlinear	2	1.36
Main_NonlinTrial3_Vid1.mov through _Vid4.mov	Updated Nonlinear	3	1.37
Main_LinTrial1_Vid1.mov through _Vid4.mov	Updated Linear	1	1.41
Main_LinTrial2_Vid1.mov through _Vid4.mov	Updated Linear	2	1.38
Main_LinTrial3_Vid1.mov through _Vid4.mov	Updated Linear	3	1.39

Two sets of four videos (reduced resolution and sped up via downsampling by $8\times$ to meet file size limitations) corresponding to the data shown in the main text Fig. 3.5A (nonlinear trial 1) and Fig. 3.5C (linear trial 1) are included as part of the Supplementary Information. The same naming convention is used as in Table 3.1, but with the suffix “_SpedUpLowRes”.

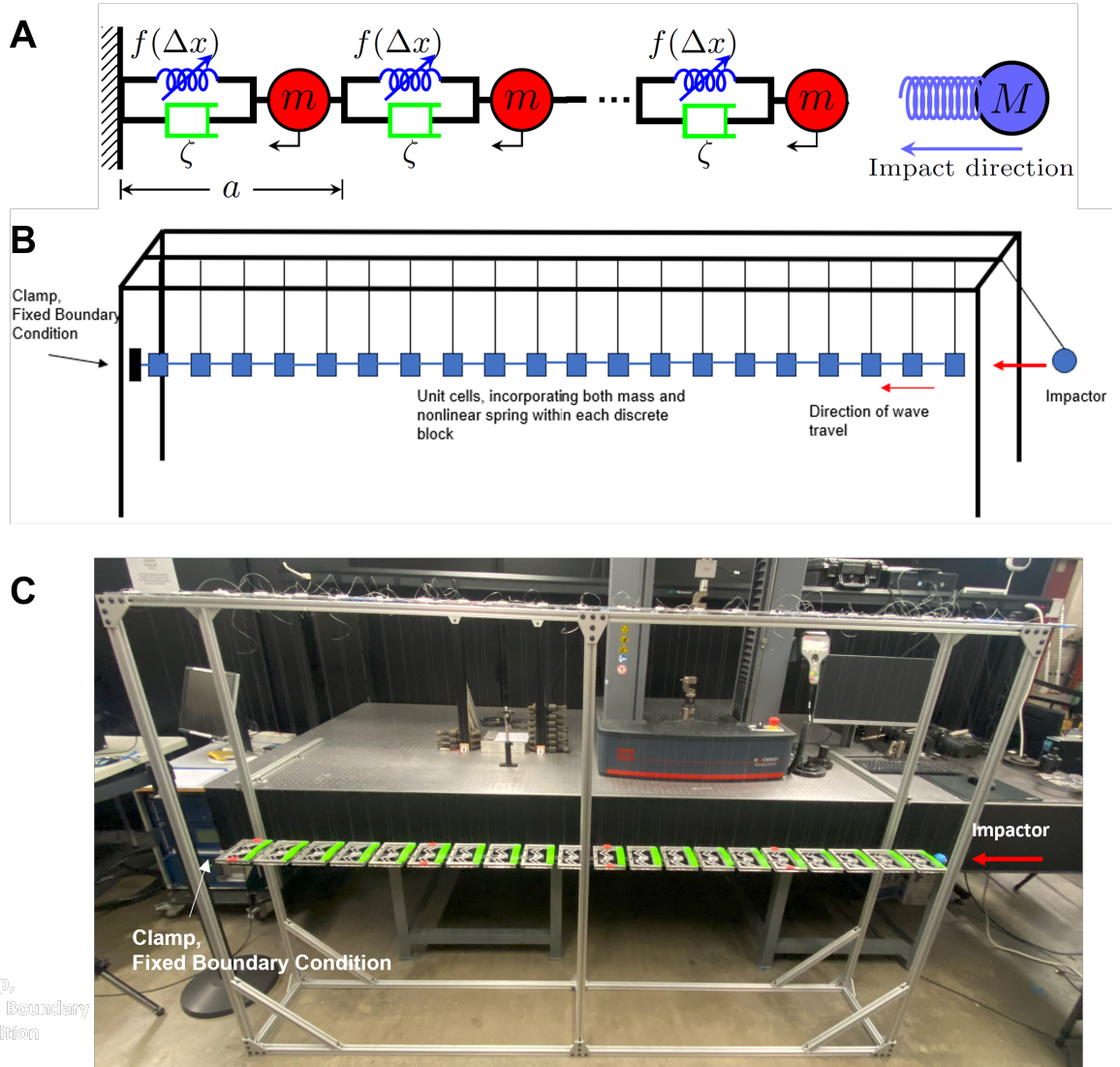


Figure 3.21. A more detailed breakdown of the experimental setup described in the main text. A) The discrete model used to simulate the system. B) A sketch of the experimental system, analogous to the model shown in A. The system is clamped on the left to impose a fixed boundary condition, while the impactor collides with the system on the right. C) A photograph of the actual experimental system, analogous with the portions in A and B. The chain shown here is the linear chain, however, we note that the setup is the same for both the nonlinear and linear chains (only the design of the unit cell varies). Note that the clamp on left edge used to impose the fixed boundary is not attached in the photo.

Included below are additional experimental data. Figure 3.23 shows the spatiotemporal kinetic energy maps from all six trials (3 nonlinear and 3 linear). Figure 3.24 contains the data gathered by the vibrometer (which measured data only from the last unit cell, unit cell 20, in

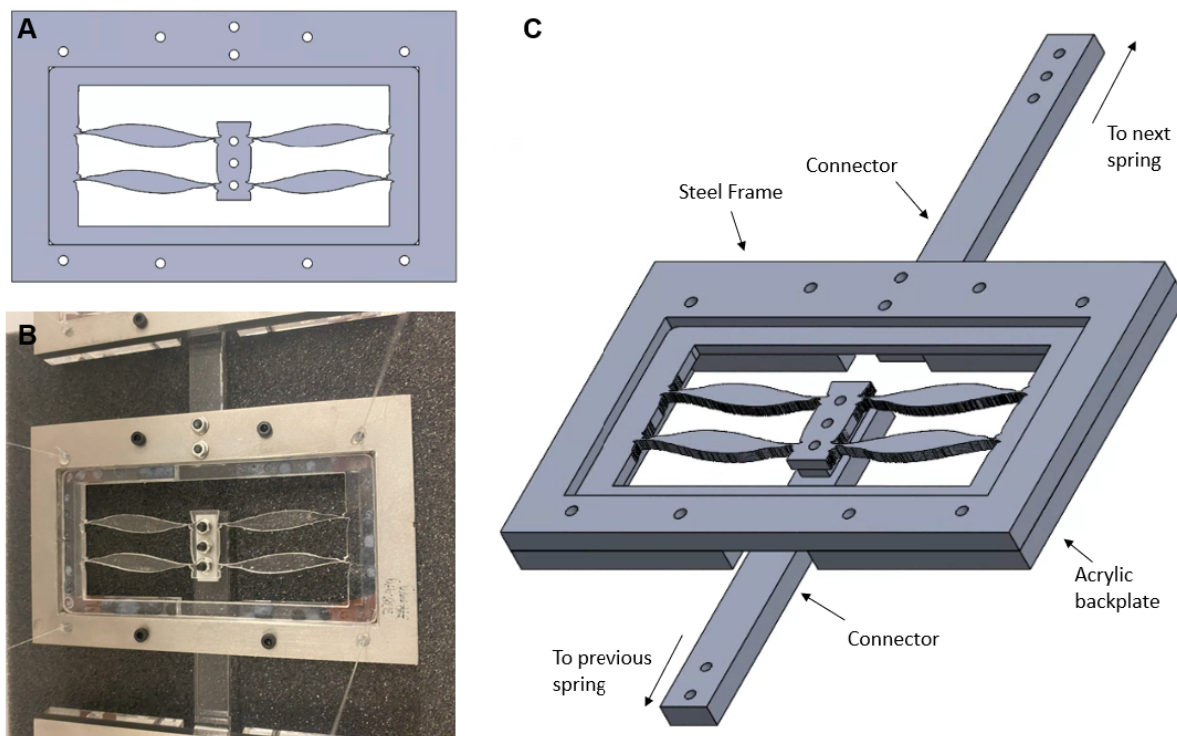


Figure 3.22. A more detailed breakdown of the unit cell design. A) A CAD model of the nonlinear spring design, embedded inside the frame. B) A photograph of one nonlinear unit cell with connectors attached. C) A CAD model of one nonlinear unit cell including the acrylic backplate and the connectors.

each chain). We note that the velocities measured by the vibrometer have been processed to account for the angle between the vibrometer and the chain (measured to be 19.35 degrees).

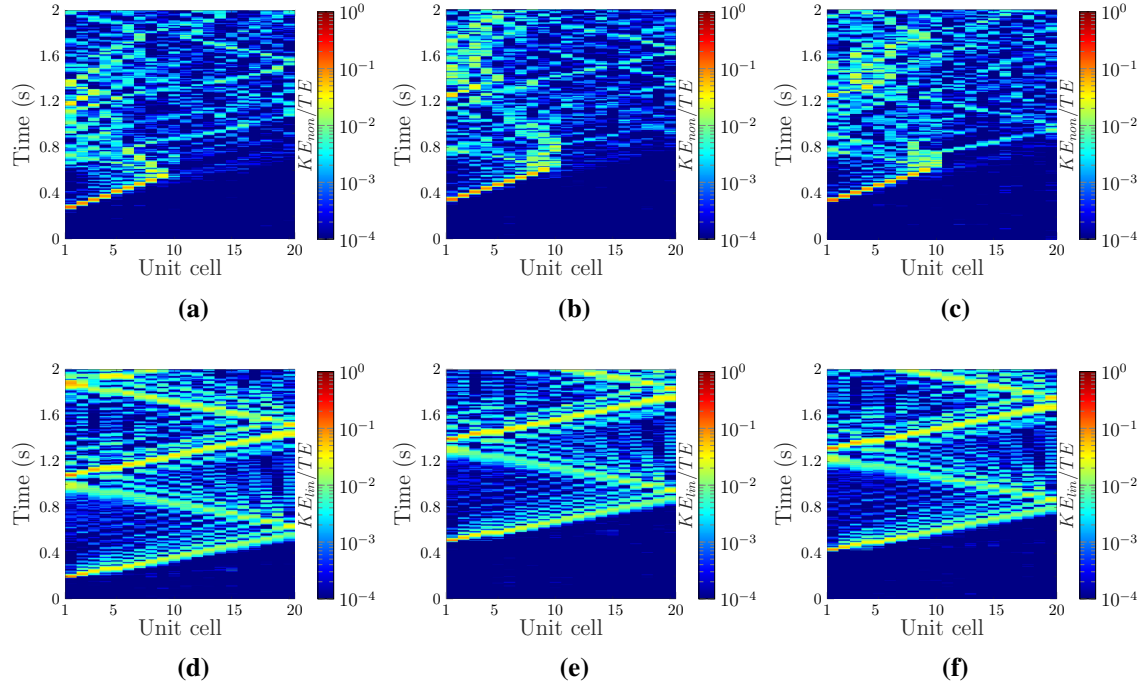


Figure 3.23. Experimental spatiotemporal kinetic energy response of the chains measured by the cameras, normalized by the input kinetic energy ($0.5MV^2$). (a-c) Nonlinear chain trials 1-3. (d-f) Linear chain trials 1-3.

In Fig. 3.25(a) and (b), we show the spatiotemporal evolution of the strain at each unit cell, $(x_{i+1} - x_i)/a$, corresponding to Fig. 3.5A and B in the main text, respectively. The strain being lower than -2.8% indicates that the spring has passed the second stable state, achieving snap-through.

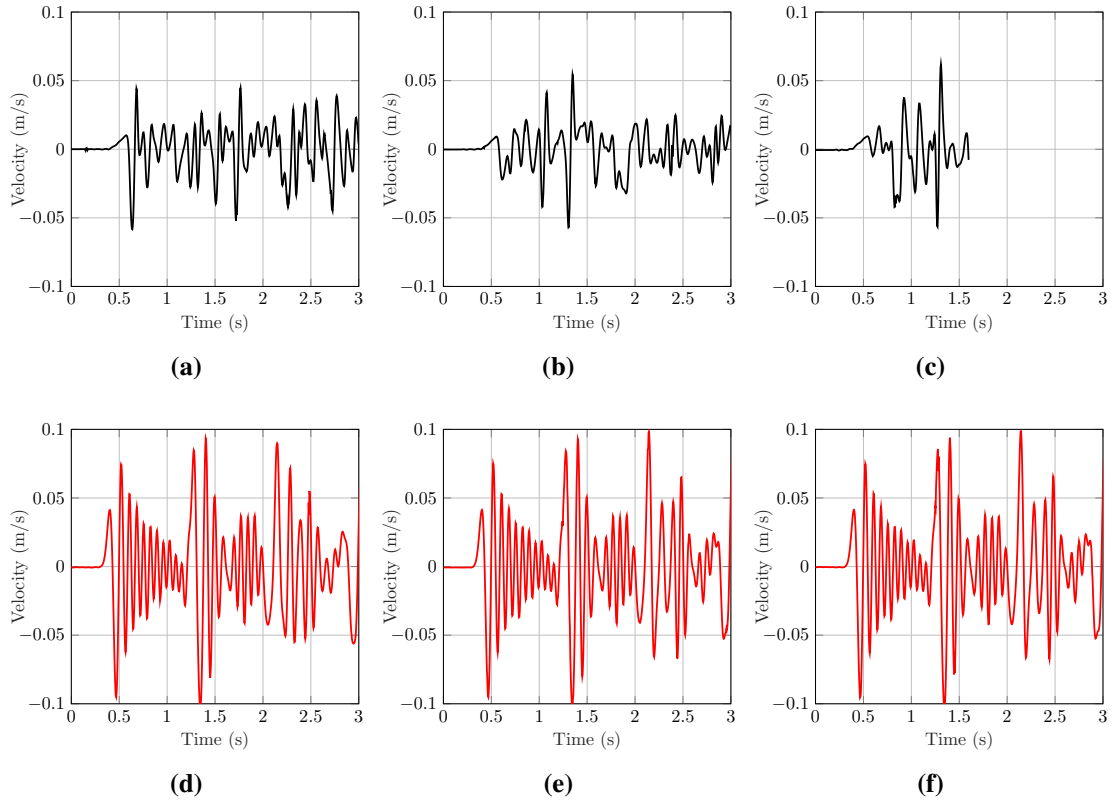


Figure 3.24. The velocity of the last unit cell of the chain, as processed from the vibrometer data to account for the tilted angle, for (a-c) nonlinear trials 1-3 and (d-f) linear trials 1-3.

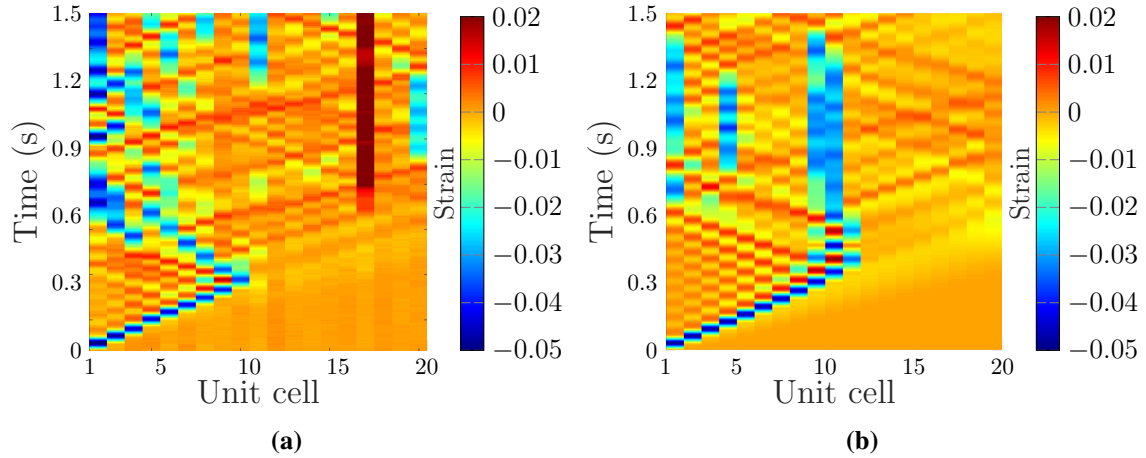


Figure 3.25. Spatiotemporal evolution of (unit cell scale) strain for the nonlinear system of Fig. 3.5A and B in the main text. (a) Experiment (corresponding to Fig. 3.5A in the main text) and (b) simulation (corresponding to Fig. 3.5B in the main text). When the strain deformation is below -2.8%, the bistable spring snaps through to the second stable state.

Note 8: Independence of kinetic energy transmission in the linear DEM chain

A non-intuitive result can be seen where changing the stiffness c_1^* of the linear undamped DEM chain does not affect the amount of kinetic energy transmitted through the chain (Fig. 3.26), keeping all other parameters constant. In Fig. 3.26, the time axis is shortened proportional to $\sqrt{c_1^*}$ to account for the faster wave speed.

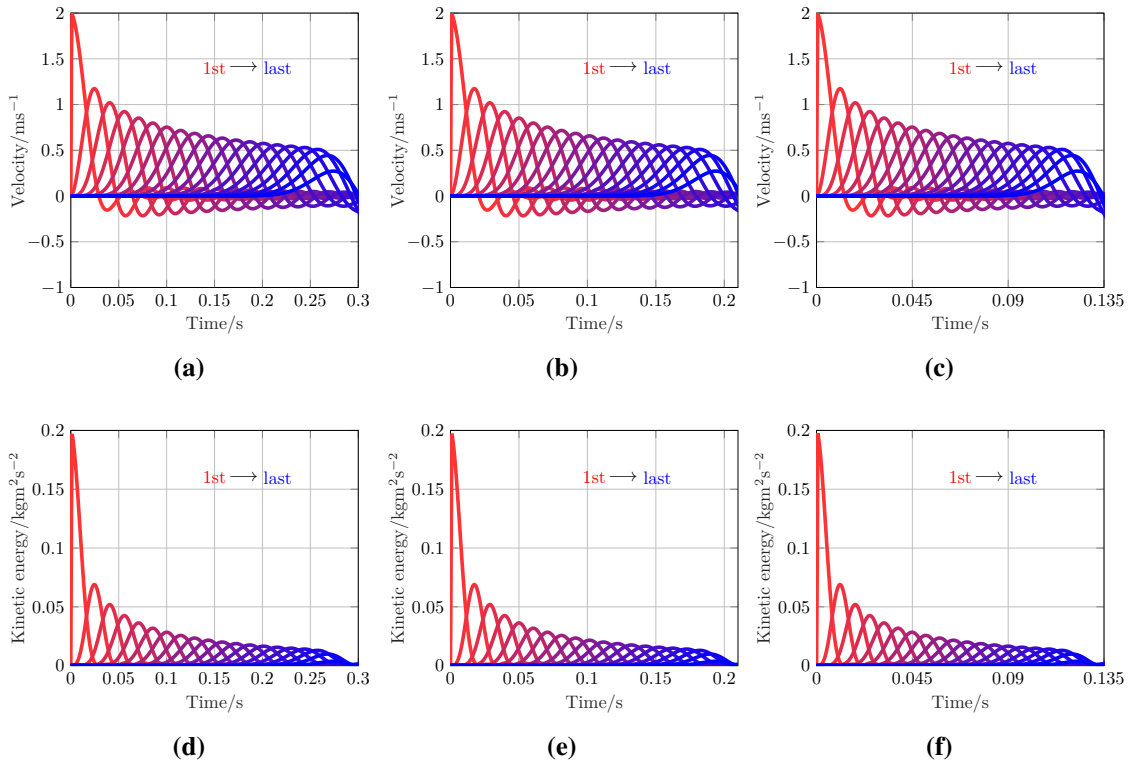


Figure 3.26. Time-velocity and kinetic energy plots for a DEM-simulated undamped linear chain with different stiffness: (a,d) $c_1^* = 500$ N/m, (b,e) $c_1^* = 1000$ N/m, and (c,f) $c_1^* = 2500$ N/m. All other physical parameters remain constant, $m = 0.1$ kg, $a = 0.1$ m, $M = 0.1$ kg, and $V = 2$ m/s.

Note 9: Additional experiments with different target coefficients

Included below are additional experimental data taken from an initial bilevel inverse design attempt (prior to that shown in the main text). In this initial attempt, we did not account for the highly oscillatory nature of the KE performance space with respect to impact conditions (see Fig. 3.5F in the main text and Fig. 3.27F below). Thus, small variations in impact velocity had significant effects upon the performance of this initial attempt, highlighting the importance of considering such sensitivity. For the design described in the main text, we took this into account, choosing an optimum with less KE sensitivity to impact conditions. As part of the redesign, we also made the unit cell larger to allow for the manufacturing of finer details in the nonlinear spring, and updated the frame from polycarbonate to stainless steel (which allowed greater stiffness with less volume).

For the initial design, the target coefficients on the unit cell scale were $f(\Delta x) = \Delta x + 94.4\Delta x^2 + 2000\Delta x^3$, corresponding to $f(\Delta x) = \Delta x_s - 30.2\Delta x_s^2 + 204.8\Delta x_s^3$ on the spring scale (with a value of $a_s = 40mm$), with a final achieved experimental fit of $f(\Delta x) = -0.0003 + \Delta x_s - 28.28\Delta x_s^2 + 193.13\Delta x_s^3$. Figure 3.27 is the analog for the initial design to the current Fig. 5 in the main text, showing experimental vs. simulation KE maps for the previous experiments, the KE ratio for the previous experiments, and the sensitivity of KE to impact conditions for the previous experiments. We note the lowered average performance in Fig. 3.27E, as compared to Fig. 3.5E in the main text.

We note the presence of several nonlinear experimental trials that are excluded from the average of Fig. 3.27E due to the onset of anomalous behavior. The videos for these additional trials are included in Table 3.2). The anomalous behavior included a unexpected increase in observed velocity values as compared to previous trials, particularly in the last unit cell, as well as, in trial 6, an unexpected spike in displacement (accompanied by a unit cell snapping) at unit cell 15, far past the number of unit cells (4-5) expected to snap through to the second stable state.

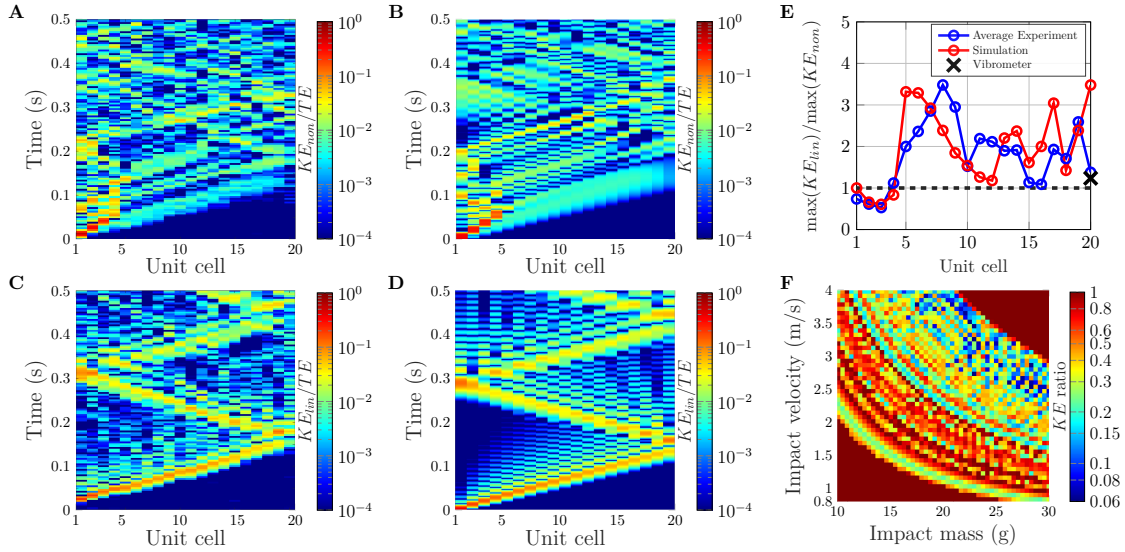


Figure 3.27. Experimental validation of the previous optimal nonlinear and linear chains, compared with simulation predictions. A-D) Spatiotemporal evolution of kinetic energy in the system (normalized by the input kinetic energy, or initial total energy). The previous nonlinear chain is shown in A (experiment, nonlinear trial 1) and B (simulation), while the previous linear case is shown in C (experiment, linear trial 1) and D (simulation). The experimental spatiotemporal plots include a smoothing of displacement values to assist with noise induced by differentiating the discrete time camera data. E) The maximum kinetic energy (linear/nonlinear) seen at each unit cell for both experiment and simulation. A value greater than 1 indicates superior performance of the nonlinear chain as compared to the linear. The experiment values are the average taken from three experimental trials. The X marks the average experimental value recorded by the vibrometer, which collected data from only the last unit cell. F) The simulated sensitivity of the KE ratio (truncated at 1) to impact conditions for the previous target coefficients.

We posit that this behavior was due in part to repeated testing of the system. Multiple trials were run before the data sets herein were collected as experimental procedures and data collection were being refined, and the excluded data were the last three trials run. This was not the case for the updated sets of experiments, presented in the main text, wherein data collection procedures had already been refined through the previous set of experiments. We hypothesize also that the unexpected spike in trial 6 may be due to either increased degradation of the spring, or fluctuating impactor velocity pushing the system into a non-ideal condition, or, perhaps, a combination of both.

Figure 3.28 shows the spatiotemporal kinetic energy maps from six trials (3 nonlinear

and 3 linear). Figure 3.29 contains the data gathered by the vibrometer (which measured data only from the last unit cell, unit cell 20, in each chain). We note that the velocities measured by the vibrometer have been processed to account for the angle between the vibrometer and the chain (measured to be 25.5 degrees).

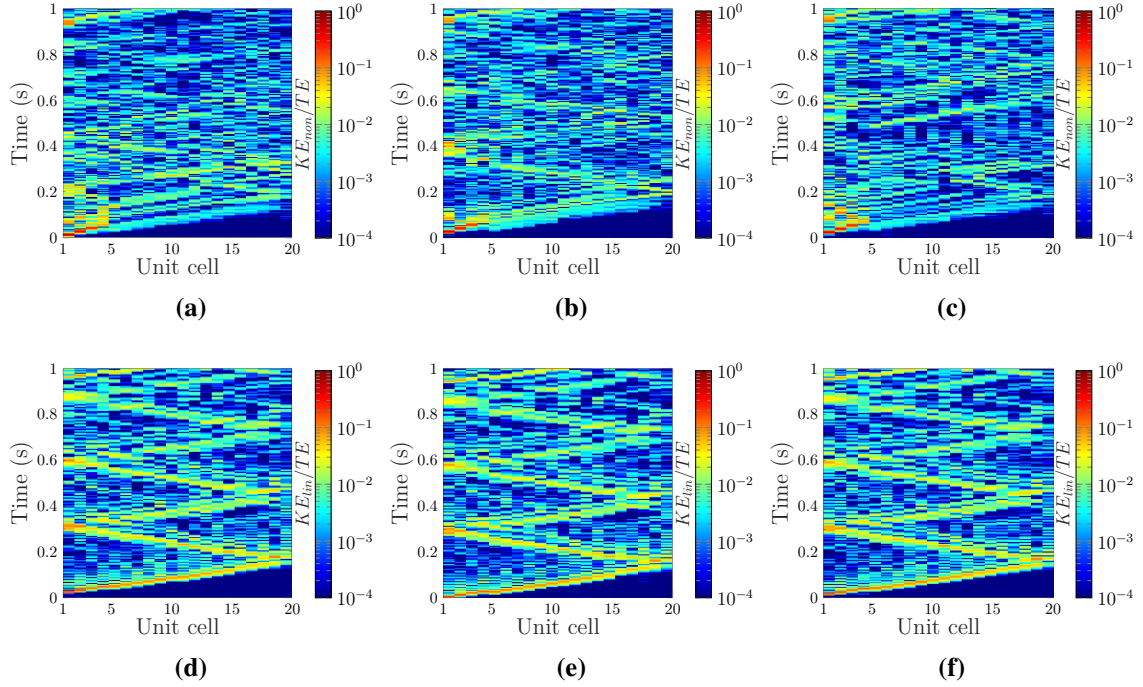


Figure 3.28. Experimental spatiotemporal kinetic energy response of the chains measured by the cameras, normalized by the input kinetic energy ($0.5MV^2$). (a-c) Nonlinear chain trials 1-3. (d-f) Linear chain trials 1-3.

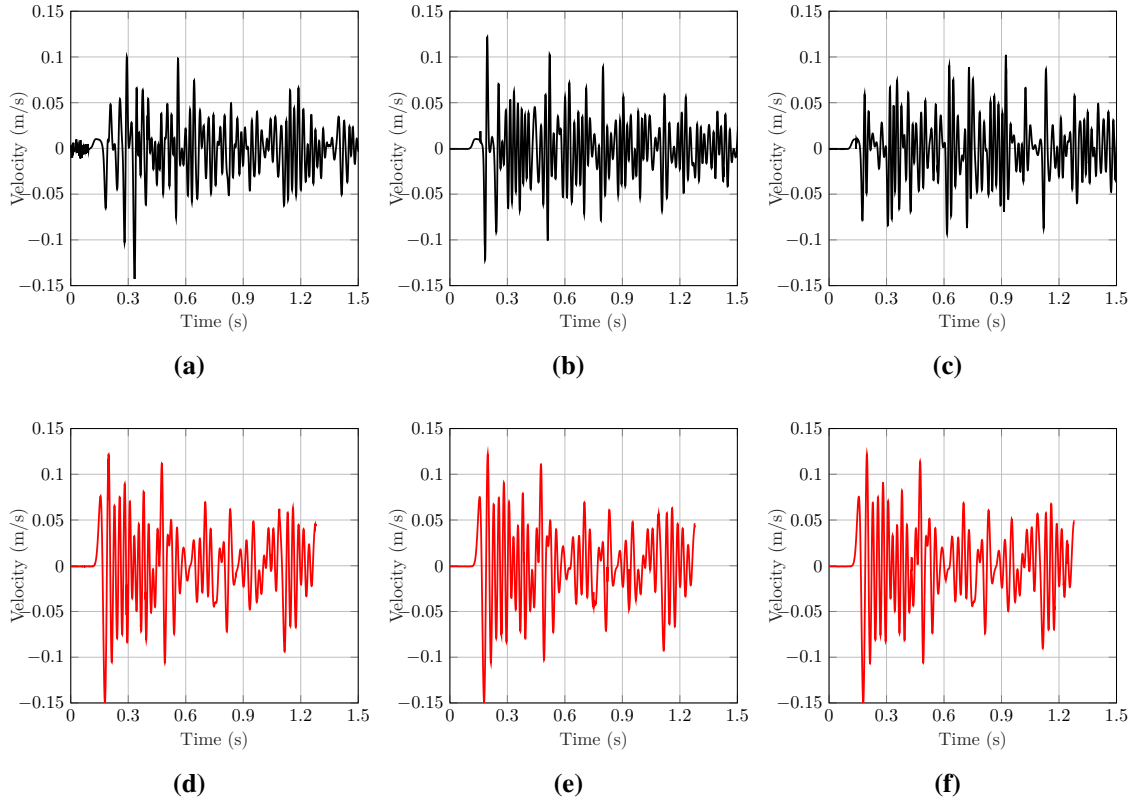


Figure 3.29. The velocity of the last unit cell of the chain, as processed from the vibrometer data to account for the tilted angle, for (a-c) nonlinear trials 1-3 and (d-f) linear trials 1-3.

In Fig. 3.30(a) and (b), we show the spatiotemporal evolution of the strain at each unit cell, $(x_{i+1} - x_i)/a$. When the strain is less than 2.8% the spring has passed the second stable state, achieving snap-through.

The videos of these previous trials are also available in the following online repository: Boechler, Nicholas (2024), “Customizable wave tailoring materials enabled by nonlinear bilevel inverse design 2”, Mendeley Data, V2, doi: 10.17632/6bg6hr5kyr.2. The details of each of these files is included in the Table 3.2 below.

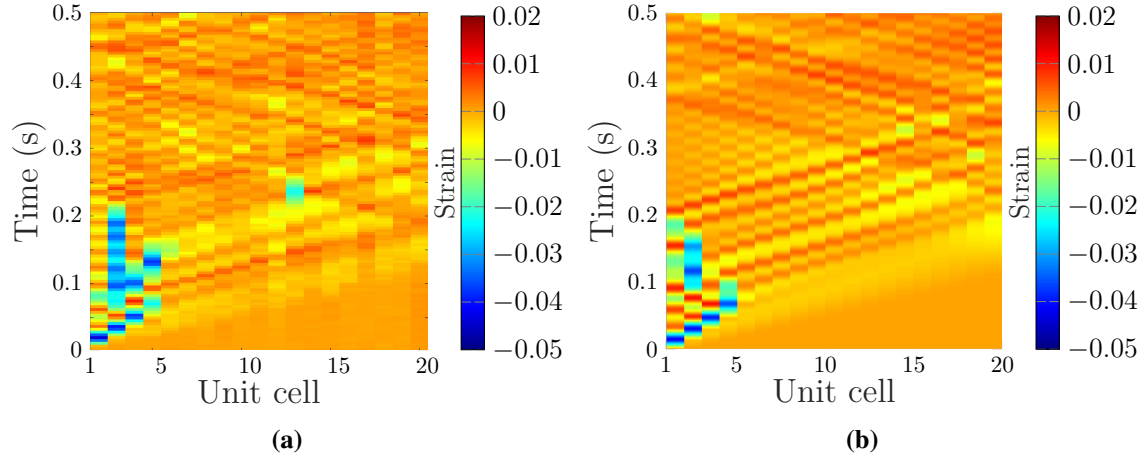


Figure 3.30. Spatiotemporal evolution of (unit cell scale) strain for the nonlinear system shown in Fig. 3.28. (a) Experiment and (b) simulation. When the strain deformation is below -2.8%, the bistable spring snaps through to the second stable state.

Table 3.2. List of previous experimentally captured video files and test details.

Video Name (1-4 for each test)	Spring Tested	Trial Number	Impactor Velocity (m/s)
NonlinTrial1_Vid1.MOV through _Vid4.MOV	Nonlinear	1	2.19
NonlinTrial2_Vid1.MOV through _Vid4.MOV	Nonlinear	2	2.10
NonlinTrial3_Vid1.MOV through _Vid4.MOV	Nonlinear	3	2.14
NonlinTrial4_Vid1.MOV through _Vid4.MOV	Nonlinear (unused)	4	2.16
NonlinTrial5_Vid1.MOV through _Vid4.MOV	Nonlinear (unused)	5	2.14
NonlinTrial6_Vid1.MOV through _Vid4.MOV	Nonlinear (unused)	6	2.11
LinTrial1_Vid1.MOV through _Vid4.MOV	Linear	1	2.23
LinTrial2_Vid1.MOV through _Vid4.MOV	Linear	2	2.20
LinTrial3_Vid1.MOV through _Vid4.MOV	Linear	3	2.16

3.6 Acknowledgements

Chapter 3, in full, has been submitted for publication. The dissertation author was one of two primary investigators and authors of this material. Authors: Brianna MacNider, Haning Xiu, Kai Qian, Ian Frankel, H. Alicia Kim, Nicholas Boechler.

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Chapter 4

Influence of strain-rate on the response of elastomeric architected materials

4.1 Introduction

Architected materials (also often referred to as “lattice” materials) have garnered significant interest [89] due to properties such as their relative high stiffness and strength at low weight, and the promise they show in energy absorption applications [188–203]. In recent years, improvements in additive manufacturing (AM) [204] methods have increasingly enabled a high degree of multi-scale tailorability in such materials. This has helped allow researchers to design material properties through control of topology and structure, resulting in “metamaterials” with extraordinary properties. For example, by controlling buckling phenomena through 2-D and 3-D ligament and node geometries in polymers, structures have been realized with controlled layer compaction or folding mechanisms under load [67, 95, 189, 190, 192, 195, 201], negative Poisson ratio [190, 194, 197, 205, 206], and high modulus-to-density (for example in stretch-dominated structures) [91, 106, 195, 203]. Multiple studies have explored how energy absorption varies with constituent material properties [91], relative density [11, 88], strut and wall thickness [11, 108], grading [102, 207], loading direction [204, 208], as well as different types of lattice geometries [11, 89, 107].

The response of architected materials in the low-to-intermediate (up to $\sim 10^4 \text{ s}^{-1}$) strain rate range has been of particular interest due to envisioned uses such as lightweight structural

components in automotive and aerospace applications, or blast and shock mitigating materials for soldier, vehicular, and building protection. This range can be thought of as a transition region where there is a potential for the behavior of the architected material to exhibit rate dependency, but the loading has not yet reached the very high strain rates where effects such as structure-independent compaction fully dominate the response. This rate dependency can be expected to manifest in two principal ways, namely constituent material rate dependency and inertial effects at higher strain rates. The onset and qualitative contribution of inertial effects to an architected material object's dynamic response depends on the relative characteristic length and time scales of the loading, confinement, material architecture, and the overall object [82]. The effect of strain rate in this regime on the dynamic behavior of architected materials has been studied in a variety of structures, including disordered structures such as foams, honeycombs, TPMS structures, ordered lattices, and lattices with modified struts [95, 192, 207, 209]. The bulk of these dynamic studies, however, have focused on metallic architected materials, rather than polymer ones or, even rarer, soft elastomeric ones. We note that many metallic lattice studies suggest constituent material strain rate dependency, with some explicitly suggesting negligible inertial effects [88–90]. Others, in contrast, report distinct inertia-induced strain rate sensitivity [104] and velocity-dependent collapse modes [92, 104, 107]. While recognizing the effects observed in metallic lattices, it is important to note that architected materials made of soft elastomers exhibit significant qualitative differences, including high ductility at large strains and viscoelastic effects. Determining the loading conditions at which strain rate begins to dominate, and the associated deformation mechanisms involved as strain rate increases, is important for predicting intermediate-to-high strain rate performance of elastomeric architected materials and designing for enhanced performance in such regimes .

In this work, we explore the $< 1 \text{ s}^{-1}$ to $\sim 10^3 \text{ s}^{-1}$ strain-rate response of four elastomeric architected materials (shown in Fig. 4.1), wherein we expect both inertial and constituent material strain rate dependence effects may play an important role. Indeed, aside from the previously described strain rate effects observed in architected materials, the soft polymeric materials we

study herein have also been shown to exhibit significant strain rate effects in this regime in bulk form [81]. Using a Split Hopkinson Pressure Bar (SHPB) [210] and a high speed camera paired with digital image correlation (DIC) [211] techniques, we demonstrate a range of behaviors that dominate the response of AM structures at varying strain rates. From the DIC data, we extract strain fields as a function of time for the dynamically-tested lattices, allowing us to track differences in deformation modes as a function of strain rate. We highlight the effect of both the constituent material properties and the length scales in determining when the transition to strain rate importance occurs, as well as the influence of the lattice geometry in the emergence of distinct deformation modes. We further offer design principles for optimizing responses at differing strain rates, based on the design aspects which determine the dominant deformation mechanisms.

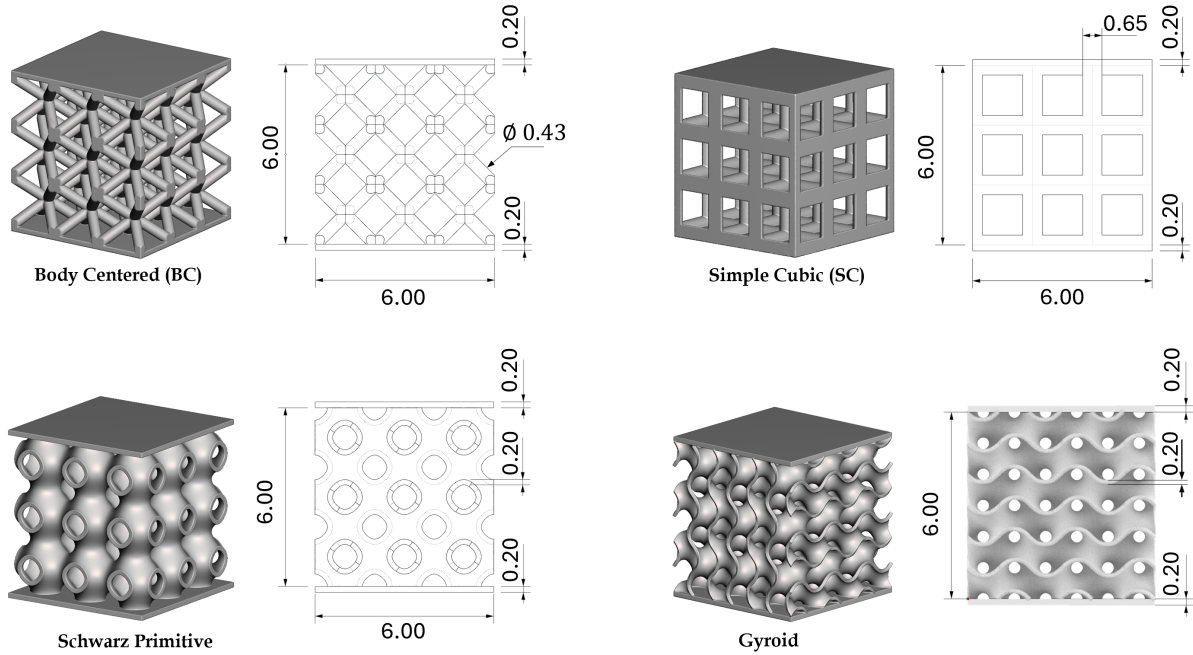


Figure 4.1. 3D models of four additively-manufactured polyurethane structures (clockwise from top left) Body Centered (BC), Simple Cubic (SC), Schwarz Primitive (P), and Gyroid (G).

Table 4.1. Dimensional details of the four additively manufactured polyurethane structures studied herein.

Structure	Outer dimensions (mm)		Strut Thickness (μm)			Structure Density ^c (g/cm ³)	Effective Elasticity Modulus
	Theor. ^a	Exp. ^b	Theor.	Exp. ^b	Difference (%)		
BC	6×6×6.4	5.6×5.6×5.4	430	459	6.7	0.472	84 kPa
SC	6×6×6.4	5.7×5.6×5.5	650	628	3.4	0.456	195 kPa
Primitive	6×6×6.4	5.7×5.5×5.4	175	201	14.9	0.561	217 kPa
Gyroid	6×6×6.4	5.6×5.4×5.3	135	181	34.1	0.718	410 kPa

4.2 Experimental

4.2.1 Materials and manufacturing method

Stereolithography (SLA) is an additive manufacturing process that uses a UV light source to cure resin in a layer-by-layer fashion to achieve the final desired 3D topology [212–215]. By adopting SLA technology, polymer structures were printed using Elastic 50A resin (Formlabs Inc.) [], a photopolymer resin classified as a polyurethane, on a Formlabs Form3+. Default printing parameters were controlled by Preform software version 3.24.2. The layer thickness was set to 80 μm , and a 0.2 mm of bulk support plate was printed on both the top and bottom, except for any internal support features. The structures were washed for 3 days in isopropyl alcohol then dried for an additional 3 days at 40 °C. Then, they were cured under UV light for 10 min at 40 °C. The solid density of the cured resin was $\rho_0 = 1.071 \text{ g/cm}^3$. Four different structures were prepared: simple cubic (SC), body-centered (BC), gyroid (G), and primitive (P). The STL files for the structures are shown in Figure 1. The theoretical (target) strut thicknesses in the print were: SC 650 μm ; BC 430 μm ; Gyroid 135 μm ; and Primitive 175 μm . Details about the sample dimensions and densities are given in Table 4.1.

4.2.2 Quasi-static compression tests

Quasi-static compression measurements were performed on samples of the same type as those outlined in Table 4.1 using via load frame testing. We note that a separate set of samples

was used for quasi-static and dynamic testing. Three tests were performed at $\dot{\epsilon} = 0.2$ mm/s to maximum stresses of 0.1 MPa, 0.2 MPa, and 1 MPa.

4.2.3 Hopkinson-bar testing

Split-Hopkinson Pressure Bar testing was performed at Los Alamos National Laboratory using an apparatus described previously [210]. Strain gauges (Dynasen, Inc.) were glued at the incident bar and sample transmission bar interface. Three firing pressures (5 psi, 10 psi, and 20 psi) were used to launch the incident bar at velocities of ~ 32.7 m/s, ~ 47.6 m/s, and ~ 62.5 m/s. Each sample had a speckle pattern applied to the surface, using spray paint, prior to testing. A Shimadzu HPV-X high speed camera (500,000 frames per second) was used to capture video of the SHPB tests, allowing for the use of digital image correlation [211] methods. Due to weak transmitted signals typical of elastomers, we focus on the DIC data obtained from these experiments and use the SHPB as a loading mechanism only.

4.3 Results

4.3.1 Quasi-static compression

Under the low strain-rate compression, the four AM structures exhibited different mechanical responses owing to the deformation and compaction mechanisms associated with their respective topologies. The resulting stress-strain curves are shown in Fig. 4.2. Optical images at several points throughout the compression test for each structure are shown in Fig. 4.3. Each sample was subjected to four consecutive loading cycles. A linear fit to the elastic region (up to $\epsilon \sim 10\%$, see SI for fits) of the first cycle stress-strain curve was used to calculate the effective elastic modulus for the structure. These values are recorded in Table 4.1.

For the BC structure a relatively linear stress vs. strain (σ vs. ϵ) response can be seen until $\epsilon \sim 30\%$. This effective modulus is relatively soft compared to the other lattices, as expected as it is a “bend dominated” lattice (referring to its connectivity being less than the Maxwell

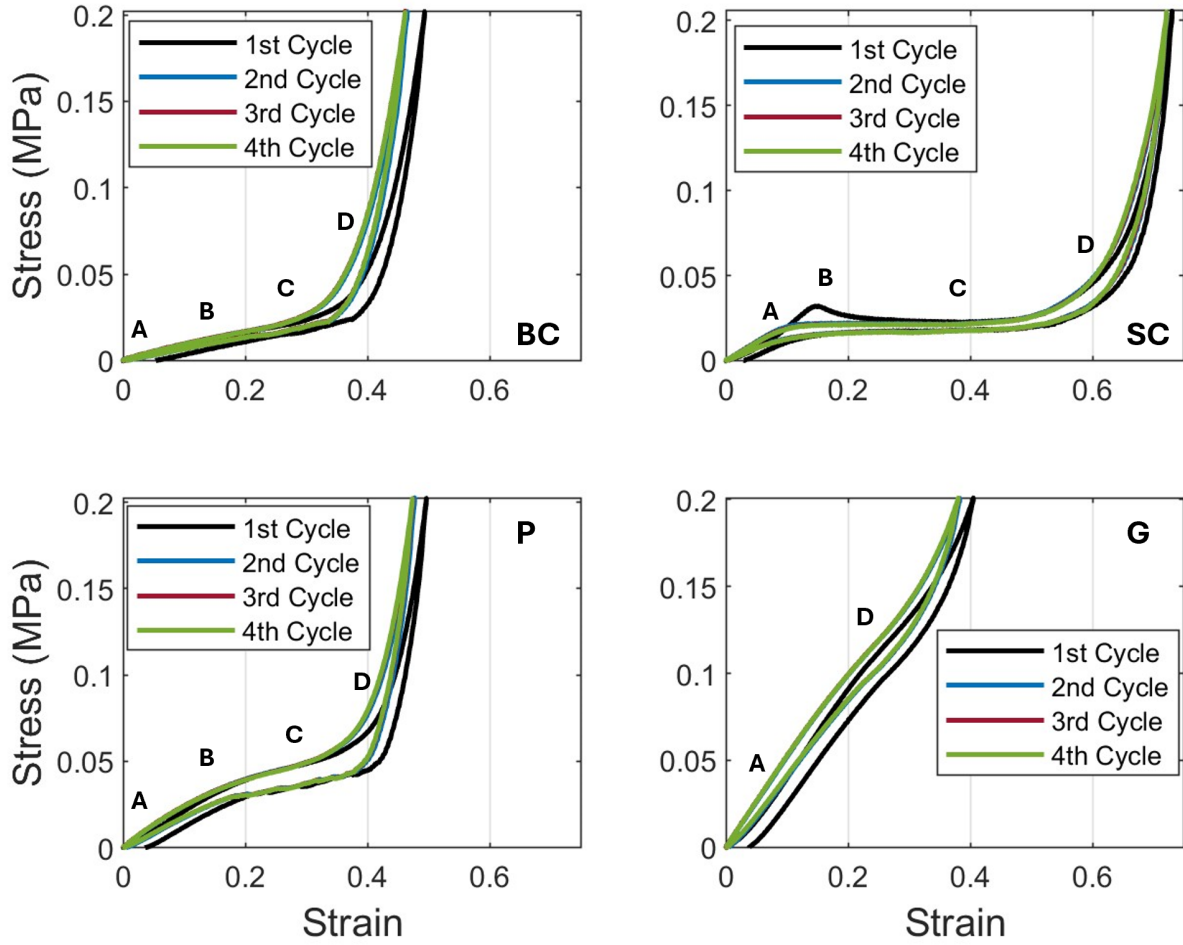


Figure 4.2. Stress-strain curves from quasi-static compression experiments to a maximum stress of 0.2 MPa. Clockwise from top left: Body-centered (BC), Simple cubic (SC), Primitive (P), and Gyroid (G) structures, are as described in the Experimental Section and shown in Fig. 4.1. The curves are annotated to describe regions of deformation behaviors: A) Quasi-elastic loading, B) Structural Yield, C) Plateau, and D) Significant structure self-contact and densification. Stress-strain curves for two additional maximum stress test values are given in the Supplementary Information.

criterion) [77, 78]. The “accordion-like” mode of deformation for this strain region can be seen in the first two panels of the top row of Fig. 4.3. At $\epsilon > 30\%$, we see a progressive densification of the lattice, shown in the third panel of the same row in Fig. 4.3, and by the significantly increased effective modulus in this strain region in Fig. 4.2a (reaching full densification at $\epsilon \sim 35\%$). Upon unloading, a small hysteresis can be observed, which may be related to either viscoelastic or plastic deformation processes. Subsequent loading cycles show roughly similar

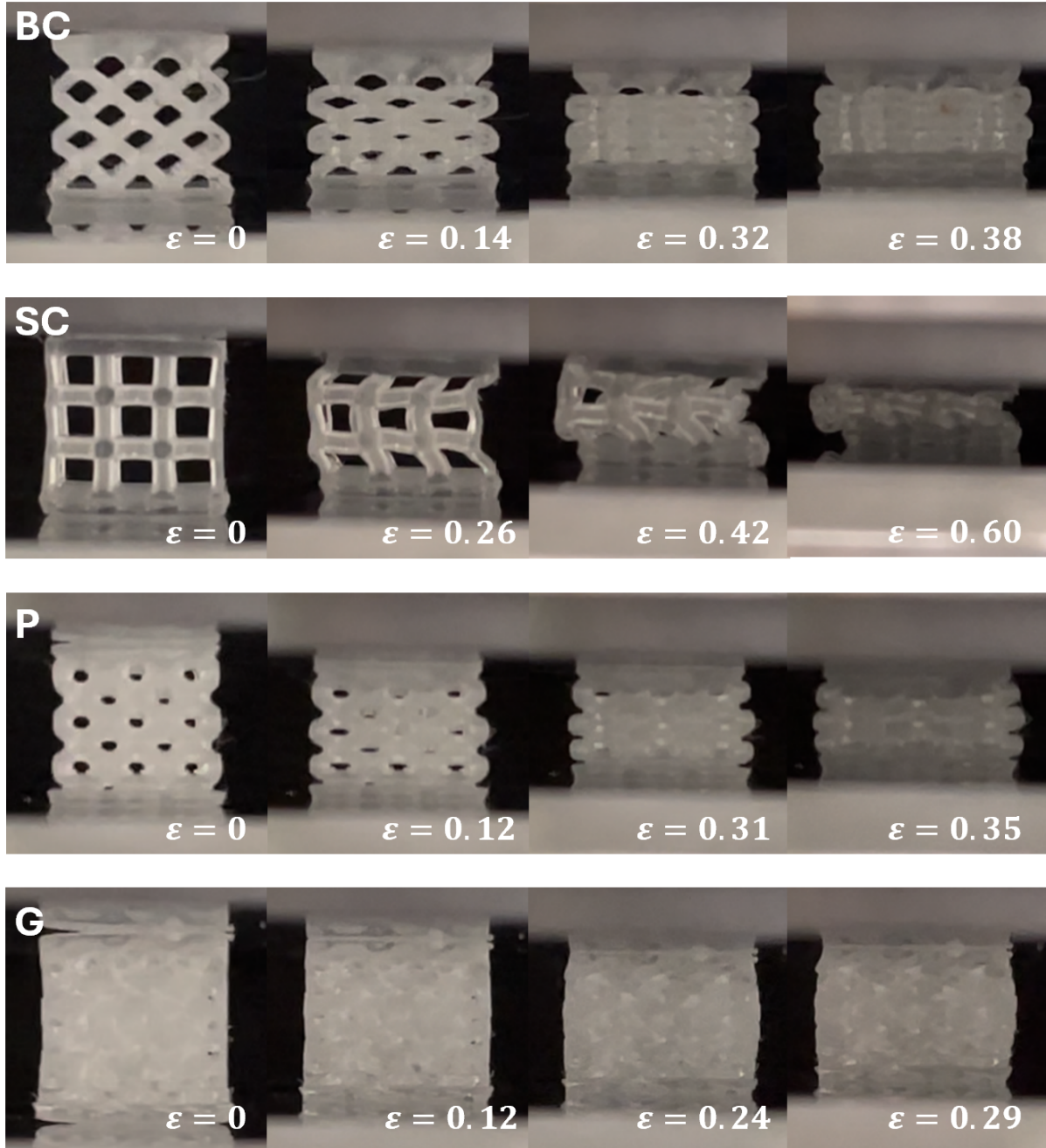


Figure 4.3. Optical images of the Body-centered (BC), Simple cubic (SC), Primitive (P), and Gyroid (G) structures (top to bottom), taken during the quasi-static compression tests shown in Fig. 4.2.

low strain behavior, but a slightly lowered densification strain.

We next consider the SC structure in Fig. 4.2b, with the corresponding deformation images in the second row of Fig. 4.3. The SC structure displayed structural instability at

$\varepsilon \sim 20\%$ resulting in buckling of the lattice elements aligned with the compression axis. The initial, pre-buckling effective modulus of the lattice can be seen to be significantly higher than the BC lattice, dropping to a near-zero modulus plateau. Further loading resulted in a continuation of the plateau until progressive densification, denoted by the rapid rise in stress at $\varepsilon \sim 50\%$ to 60% strain. In contrast to the BC lattice, a qualitative behavior change can be seen after the first loading cycle, where the clear peak in stress around $\varepsilon \sim 15\%$ disappears, which suggests at least some local irreversible process (either plasticity or fracture), although the total permanent strain retained after unloading is still minimal.

The P structure at first displayed a nearly-linear behavior of similar stiffness to the SC lattice (*i.e.* stiffer than the BC structure), as seen in Fig. 4.2c and the first two images in the third row of Fig. 4.3. It began to exhibit softening behavior around $\varepsilon \sim 20\%$ as the voids changed shape and began to collapse. Significant densification begins to occur in the $\varepsilon \sim 30\%$ to 40% range (right two images in the third row of Fig. 4.3), marked by a shift to stiffening behavior, quickly followed by a sharp rise in stress in the $\varepsilon > 40\%$ region. Similar to the BC structure, in subsequent loading cycles we observe very similar behavior at lower strains, but a slightly lowered densification strain (closer to the lower end of the $\varepsilon \sim 30\%$ to 40% range).

The high initial density (low porosity) of the G lattice (see Table 4.1) resulted in earlier (relative to the other structures) ligament contact and densification, leading to much stiffer initial behavior, as seen in Fig. 4.2d. The structure can be seen to maintain a quasi-linear behavior until $\varepsilon \sim 20\%$ (left two images of the bottom row of Fig. 4.3), followed by a period of weak softening until $\varepsilon \sim 30\%$. This softening region is accompanied by a bulging outward of the sides of the structure, as seen in the right two images of the bottom row of Fig. 4.3. This slight softening is followed by a shift back to stiffening at $\varepsilon > 30\%$. Subsequent loading cycles result in a shift to the left of the entire curve, again suggesting irreversible processes.

The specific energy absorption [216] of each lattice, taken as the area under the initial load-displacement curve divided by the mass of the structure, is calculated to range from 58.16 J/kg (SC), to 50.58 J/kg (G), to 44.59 J/kg (P), to 36.76 J/kg (BC). The ability of the SC structure

to accommodate large strains via structural yielding gives it the highest quasi-static specific energy absorption.

4.3.2 Hopkinson-bar experiments

For the previously-described SHPB experiments, DIC analysis was performed on the recorded video using the program VIC-2D. Strain fields and displacements were obtained through this analysis, and further processed in MATLAB. Snapshots of the deformed samples at the time of maximum compression are shown in Fig. 4.4, along with the overlaid strain field in the x direction (ϵ_{xx}) obtained from DIC. The impactor is incident from right to left. The transmission bar on the left acts nearly as a rigid boundary due to the limited energy transmitted. It can be seen that increasing the input pressures results in successive increases in global compression (top to bottom rows). This, along with the corresponding increasing strain rate, results in the activation of different deformation mechanisms and different regions of the stress-strain curves as a function of both lattice type and strain rate.

In Fig. 4.4, the BC lattice, all strain rates show a smooth collapse of local features from the right to the left, which is indicative of wave-like behavior. As the strain is increased to 2500 s^{-1} and 3000 s^{-1} (middle and bottom rows), self-contact is made between local features (shown in the bottom two BC rows in Fig. 4.4), engaging the region of maximum compression (the region marked D on the quasi-static curves shown in Fig. 4.2).

For the SC lattice, we observe at all tested strain rates that deformation of the voids begins with localization at the right edge (close to the impactor) that propagates to the left edge. At $\sim 1500 \text{ s}^{-1}$ (top), we note the onset of localized strut buckling/collapse at the left (next to the transmission bar), as indicated by the red arrows in the second column of Fig. 4.4. This could be indicative of dynamic buckling, given the observed initial localized deformation on the right, and may be consistent with stress doubling that occurs at a rigid boundary during wave propagation, wherein the threshold for local buckling may not be reached during the initial transit of the dynamic stimuli across the material. However, this may also be indicative of a more, global,

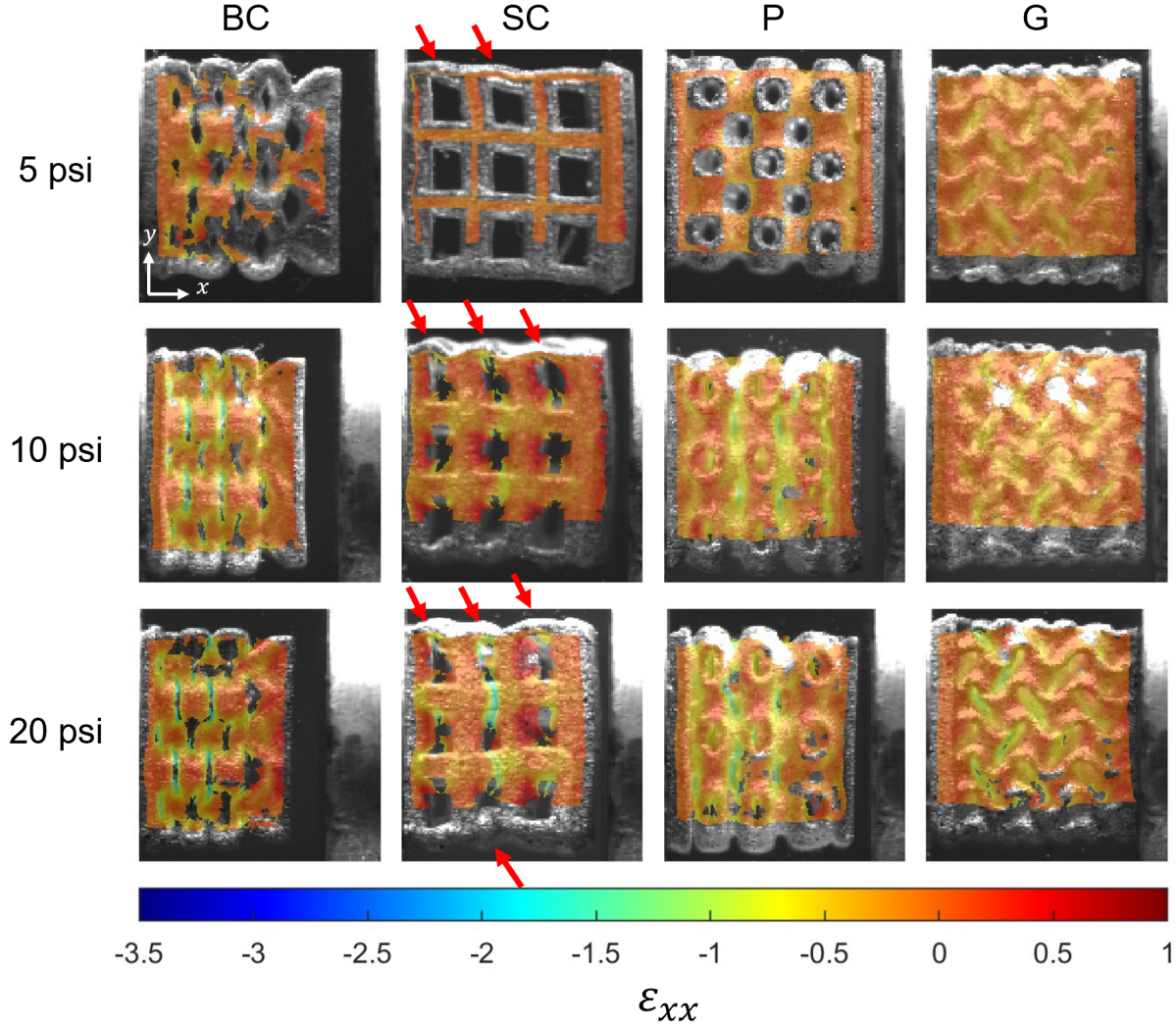


Figure 4.4. Still images of deformed lattice samples from 12 different tests at the time of maximum compression, with the DIC-calculated x-direction strain field (ϵ_{xx}) layered on top. The tests pictured are of Body-centered (BC), Simple cubic (SC), Primitive (P), and Gyroid (G) lattices (left to right columns), and 5 psi, 10 psi, and 20 psi of input pressure (top to bottom), corresponding to ~ 1500 , ~ 2300 , and $\sim 2800 \text{ s}^{-1}$ strain rates, respectively. Red arrows highlight localized buckling.

]

quasi-static buckling process due to a heterogeneous strain field, wherein the initial buckling of one location relieves stress elsewhere. No uniform or long-wavelength global buckling was seen, in contrast to the quasi-static compression tests (e.g. the second panel from the left for the SC lattice in Fig. 4.2). As the rate is increased further to $\sim 2300 \text{ s}^{-1}$ and $\sim 2800 \text{ s}^{-1}$ we observe more localized strut buckling (denoted by the red arrows), some of which is out of the

2D camera plane (highlighted by the bottom red arrow in the second column of Fig. 4.4). We suggest that the distribution of the localized buckling without apparent self-contact suggests a dynamic buckling process is occurring.

The P and G lattices both exhibit localized deformation of their features which begins concentrated at the right edge and propagates left, eventually settling to a quasi-even distribution across the sample. A change in pore shape is observable in the P lattice, at the two higher strain rates tested, which is consistent with the quasi-static tests and the measured strain fields.

4.4 Discussion

In this study, we directly compare the deformation mechanisms of several common lattice topologies engaged at strain rates on the order of $\sim 10^3 \text{ s}^{-1}$, with their responses under quasi-static compression. We are interested in studying if, where, and why a ‘transition’ region might occur, in which the deformation mechanisms shift from those observed in low strain-rate regimes to those in high strain rates regimes. Such details then may be translatable to qualitative design principles for application of hierarchical materials in dynamic loading regimes.

We note that there are two distinct effects that depend upon strain rate which could influence the behavior of the lattice. The first, the strain rate sensitivity of the constituent material, is straightforward, and is influenced principally by the choice of the constituent material and its strain rate-dependent properties. This includes effects such as viscoelasticity or thermal softening, and has been observed in many dynamic lattice investigations [95]. For the material in this work we expect that, due to the damping coefficient ($\tan \delta$) for polyurethane being on the order of $\sim 10^{-1}$ [217], that at the strain rates tested herein there will be some dynamic, viscoelasticity driven stiffening [81]. This effect may interplay with the architected material’s structural geometry, wherein strain localization can lead to locally greater strain rates and thus locally greater viscoelastic effects. The onset of inertial effects also depends not only upon the behavior of the material, but also upon the geometry. We consider that inertial effects tend to

take prominence when a ‘wave dominated’ regime is entered, which we define as occurring approximately when the distance the wave has traveled (effective pulse length) is less than some characteristic structural length scale. Outside of this regime, equilibrium is reached across the length of the sample during loading without any dynamic localization. The onset of the wave dominated regime can be described by the equation

$$\lambda < L \quad (4.1)$$

in which λ is the effective pulse length and L is the characteristic structural length scale. If we take strain rate to be

$$\dot{\epsilon} = \frac{\delta}{Lt}, \quad (4.2)$$

where δ is the displacement of the striker bar at some time t , then the condition for wave localization to arise can be written as

$$\frac{c\epsilon}{\dot{\epsilon}L} < 1 \quad (4.3)$$

assuming $\lambda = ct$, c is the effective speed of sound in the material. We henceforth refer to the nondimensional quantity $\frac{c\epsilon}{\dot{\epsilon}L}$ as the localization parameter, l .

In this dimensionless localization parameter, l , the speed of sound, c , is the effective speed of sound of the architected material. It thus incorporates not only constituent material effects, but also structural effects arising from the geometry of the lattice. Length L can be taken to be the length of the undeformed lattice, in which case localization should induce the onset of inertial effects globally, but the structure can still be approximated as a continuum. Alternatively, L can be taken as the unit cell length scale, in which case continuum approximations break down and inertial effects within the unit cell gain importance. This length scale influence is similar to the higher strain rate length scale dependent rarefaction wave interactions seen by Dattelbaum et

al. [114] in polymer fractal structures under shock loading, as well as considerations noted by Liu et al. [104] regarding metallic cellular foams. The parameter l can aid in judging if a given lattice of a given material can be expected to experience inertial effects arising from wave-driven behavior at a given strain rate. We note, for example, that many of the experiments in literature which report not seeing inertial effects at strain rates similar to those tested herein [88, 208, 209] investigated metallic lattices, which have a much higher effective speed of sound than the soft elastomeric lattices tested herein. This would result in a higher value of l , and therefore under similar loading conditions, we would expect wave effects to gain importance at lower strain rates in the lattices tested here than in similar metallic lattices.

The normal strain fields along the direction of loading (x) are one metric by which wave localization can be examined experimentally. Periodic strain across the length of the sample, commensurate with the unit cell period, would be generally expected when not in a wave-dominated regime [95, 104]. The exception to this would be the presence of mechanical instability, which may cause stochastic localized sequential buckling [218]. Alternatively, when the loading induces a wave dominated regime, we expect increasingly non-uniform global strain, concentrated at one edge and moving in the direction of the loading pulse, from which inertia-driven modification of the lattice behavior may arise.

To more easily compare ϵ_{xx} , the strain field was summed vertically over the width of the sample (transverse to the loading direction), allowing for visualization as a line representative of the strain field across the x -dimension (noting that x is the loading direction), as shown in Fig. 4.5. In the case of the SC lattice, which has relatively large voids that introduce some noise to the DIC values, strain values overlapping the edges of the voids were removed to smooth the data. This data was then plotted for each experiment to examine the ways in which localization and deformation mechanisms shift as a function of topology and strain rate. Figure 4.5 shows the 5 psi input pressure cases, with early time steps isolated, while the other test cases and times can be found in the SI. As seen in Fig. 4.5, early time steps in these strain fields clearly show an initial localization of strain on the right (impacted) edge, which then propagates to the left across

the sample as the pulse travels across the sample. This non-uniform strain is a clear indication that a wave-dominated regime has emerged, even at the lowest strain rate tested ($\sim 1500 \text{ s}^{-1}$).

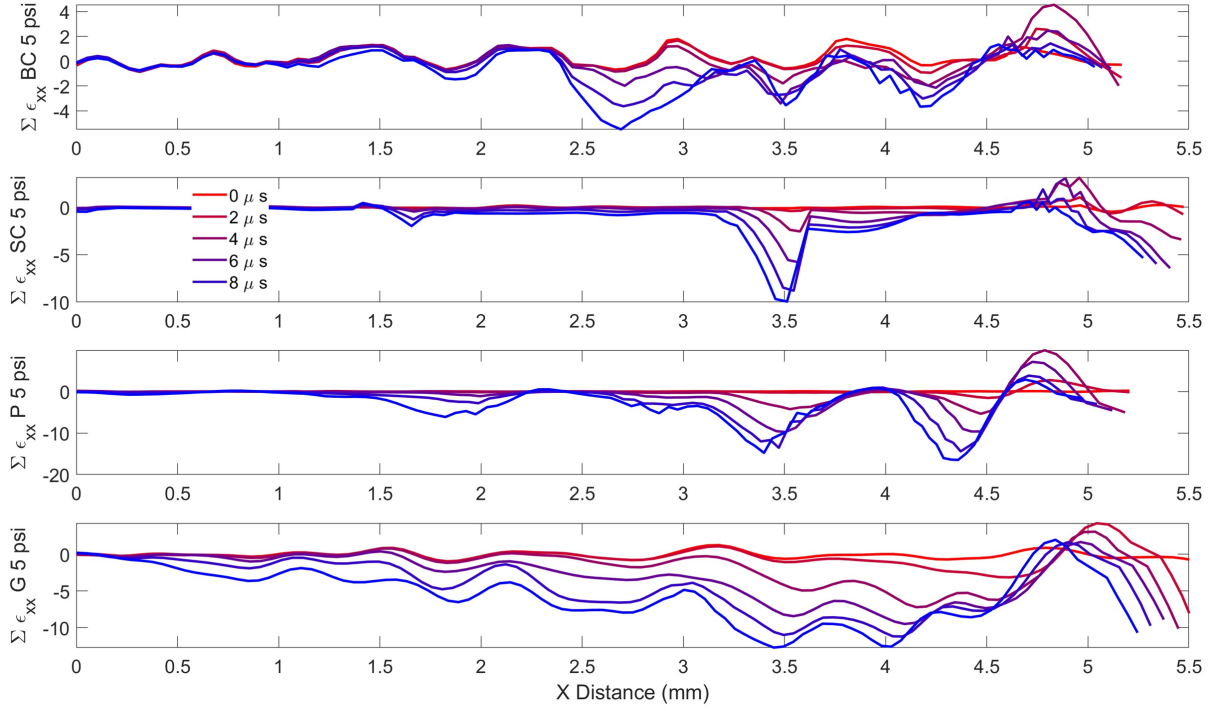


Figure 4.5. The time evolution of strain in the x direction, summed vertically over the height of the sample, in which the color shift from red to blue indicates advancing time. Data shown are for the first five frames from impact ($0 - 8 \mu\text{s}$, as outlined in legend) for A) BC lattice tested at 5 psi, B) SC lattice tested at 5 psi, C) P lattice tested at 5 psi, and D) G lattice tested at 5 psi. The same data for other test pressures, as well as the time evolution for all cases, can be found in the SI.

We can estimate the approximate speed of sound values in each structure from the quasi-static behavior, calculating the effective speed of sound as we would in a solid with the equation $c = \sqrt{(E/\rho)}$, in which E is the effective elastic modulus (values can be found in Table 4.1). Using these effective sound velocities, we can estimate the values of the localization parameter $l = \frac{c\epsilon}{\epsilon L}$. These values are included in Table 4.2. The localization parameter estimates indicate that all cases tested herein are well within the wave dominated regime, with the highest localization upper limit being on the order of ~ 0.16 , well below unity. For comparison, if the modulus E and density ρ were scaled to the range of metals (roughly 68 GPa and 2.7 g/cm^3 for Aluminum, for

Table 4.2. Magnitude and duration of impulse, associated strain rates, and localization estimates from SHPB experiments on the 4 structures.

Sample	Pulse Magnitude (ϵ) (5 psi, 10 psi, 20 psi)	Pulse Durations (μs) (5 psi, 10 psi, 20 psi)	Strain Rates (s^{-1}) (5 psi, 10 psi, 20 psi)	Max Average d (5 psi, 10 psi, 20 psi)	Estimated upper limit c (m/s)	Estimated upper limit $\frac{c\epsilon}{\dot{\epsilon}L}$ (5 psi, 10 psi, 20 psi)
BC	0.06, 0.10, 0.12	0.52, 0.53, 0.55	1500, 2500, 3000	0.055, 0.182, 0.203	13.1	0.088, 0.090, 0.095
SC	0.06, 0.09, 0.11	0.53, 0.52, 0.56	1500, 2300, 2800	0.023, 0.096, 0.153	19.1	0.131, 0.134, 0.139
P	0.06, 0.09, 0.11	0.52, 0.52, 0.55	1500, 2200, 2800	0.046, 0.089, 0.105	19.2	0.123, 0.125, 0.134
G	0.06, 0.08, 0.11	0.52, 0.53, 0.55	1500, 2100, 2800	0.032, 0.049, 0.067	25.4	0.160, 0.153, 0.156

example), and the same structures, strains, and strain rates were considered, the same estimates would put the localization parameter in the range of 10 - 20. We show the relative position of our experiments, and the estimates for aluminum analogs, with respect to $l = 1$ in Fig. 4.6. In addition to the effect of the material, we can see the effect of the structure on the effective speed of sound in the travel time of the initial pulses. The G structure, for example, is the densest (and therefore stiffest) of the samples tested, and therefore has the highest effective c value. This is consistent with the known loss of relative stiffness in low density lattice materials. In the strain data shown in Fig. 4.5, the pulse in the G structure can be seen to reach the left edge of the sample faster than the pulses in the other structures. Because of this, although the G structure is still in the wave-dominated regime, the BC, SC, and P structures are more firmly in this regime (lower localization parameter values) due to the structure leading to a shorter effective wavelength.

With regard to the mode of deformation, one of the most notable differences between the quasi-static and dynamic tests is the appearance of dynamic inertial stabilization in the SC lattice.

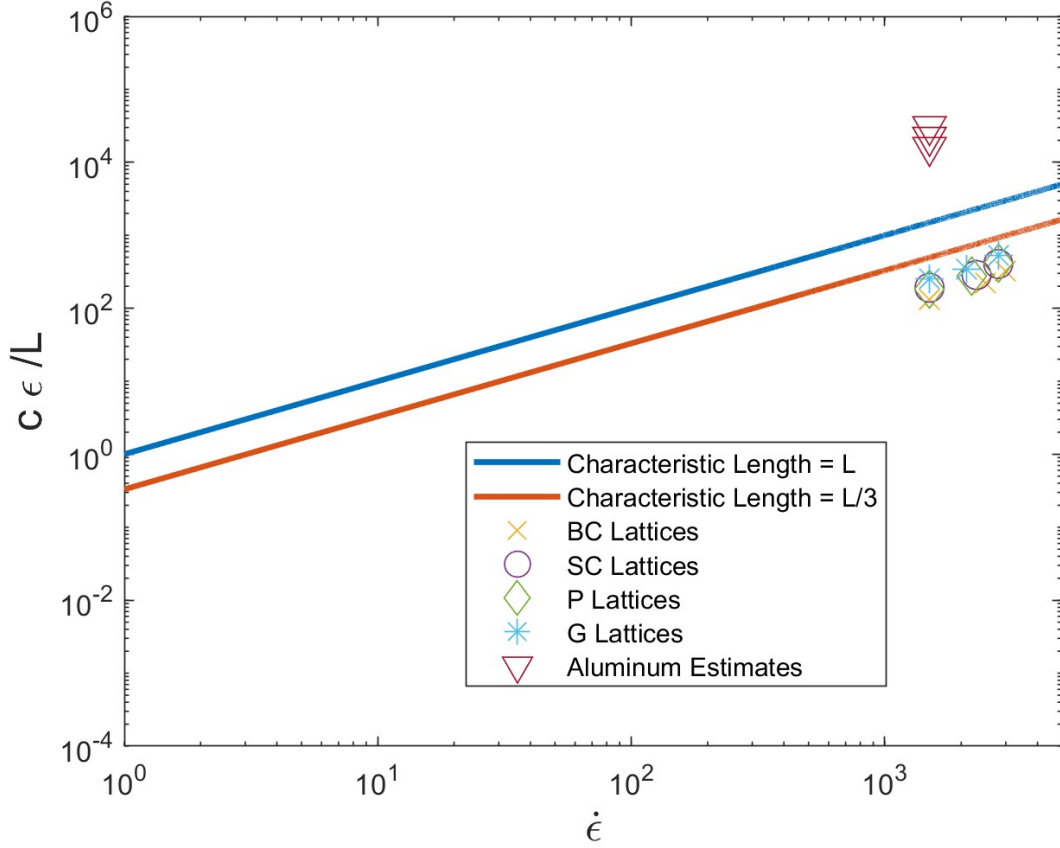


Figure 4.6. Three terms of the localization parameter plotted against strain rate. Solid lines represent the threshold across which wave localization occurs for differing characteristic lengths, with the data points from this work additionally highlighted.

Under quasi-static compression, a global, long wavelength, asymmetric buckling mode becomes energetically favorable at low strains (see Figs. 4.2 and 4.3). When dynamically compressed, particularly at the higher strain rates, we see a shorter wavelength, periodic, and globally axially symmetric, buckling mode appear. These local modes are triggered despite the tendency for the global buckling mode to be more energetically favorable, due to the shorter pulse length (*i.e.* wave dominated localization) present in the dynamic loading scenario - a well-known phenomenon in dynamically buckling beams [99, 100]. It is worth noting that this dynamic buckling has implications for the impact mitigation performance of the structure, as the onset of dynamic buckling has been shown to stabilize buckling, delaying its onset and allowing for

the support of greater axial loads up to higher displacements than would occur quasi-statically [99, 100]. Indeed, lateral inertia of the buckling elements has previously been shown to play a role in strain rate sensitivity [96, 104, 106, 219]. The higher two dynamic strain rates tested, and potentially the lower strain rate tested, demonstrated inertial stabilization and localized dynamic buckling for the SC lattice, further highlighting the onset of a regime in which inertial effects have begun to gain importance.

To explore the differences in deformation modes and localization between geometries quantitatively, the gradients of the strain fields were examined. Gradients were taken with respect to the deformed x-coordinates, smoothed, and the absolute value was taken to avoid positive and negative strains canceling out. Gradients were then averaged over the entire sample for each time (see SI). The maximum averaged gradient values from each test are summarized in Table 4.2 and plotted in Fig. 4.7, in which it can be seen that, as expected, strain localization tends to increase as strain rate and maximum overall compressive strain increases. It can also be seen that the localization of deformation is highest in the BC type topology, likely due to a combination of its relatively low density and initial low stiffness. This is followed by the SC and P type lattices, which have roughly similar localization values, and the G type lattice (which densifies quickly, as per the quasi-static plots shown in Fig. 4.2) has comparatively very low deformation localization. Of note, the SC lattice is the only topology which retains a relatively high increase in localization from the middle to the highest strain rate (see SI and Table 4.2). While the BC lattice has overall higher deformation localization, the jump from the middle to the highest strain rate is low compared to the jump the SC lattice exhibits. The P and G lattice also have reduced mid-to-high strain rate localization jumps (although we do note that, due to the 3D properties of these lattice types, and the fact that some voids are not visible in our 2D DIC capture, this may be somewhat underestimated). This difference in localization jump appears to be the result of the BC, P, and G lattices all approaching contact, or maximum compaction, regions, at which point local deformation mechanisms, and therefore topology-driven differences, have reduced importance. Meanwhile the SC lattice, both dynamically and quasi-statically tested,

does not reach compaction within the strains tested in the SHPB. This trend also aligns with expectations arising from the quasi-static stress-strain curves shown in Fig. 4.2, in which the computed specific energy absorption [216] values point to the SC lattice having superior energy absorption capacity, followed by G, P, and finally BC. It is worth noting that these stress-strain curves are expected to shift as different deformation mechanisms are engaged at different strain rates (particularly in the case of the inertially stabilized SC lattice).

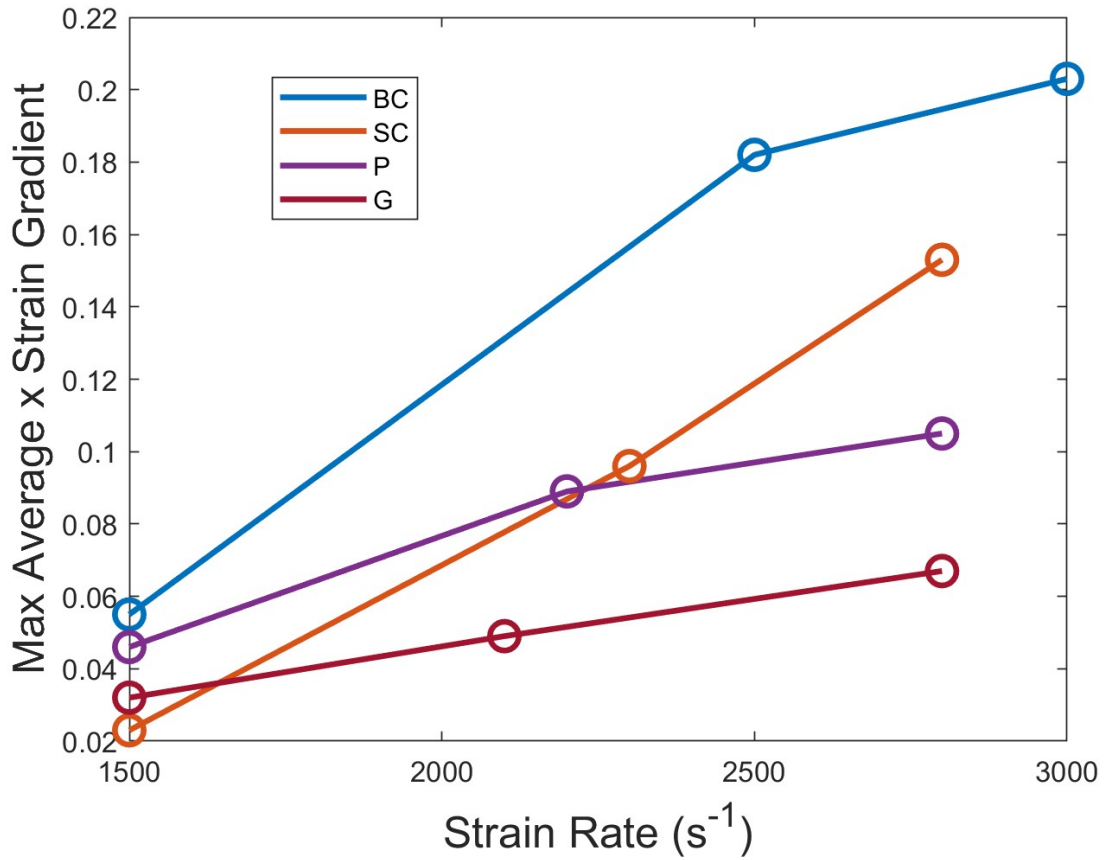


Figure 4.7. The maximum value of the average strain field gradient $\frac{d\epsilon_{xx}}{dx}$ as a function of strain rate.

In the context of examining the effects of geometry upon not only the energy absorption capabilities and deformation mode, but also the strain rate sensitivity, of a structure, we highlight that the deformation behavior of the SC lattice shows marked differences from the other three lattices in both its strain rate-dependent deformation and deformation-localization jump. We

suggest that these differences arise in large part due to the SC lattice being a ‘Type II’ geometry, while the BC, G, and P lattices can be classed as ‘Type I’ geometries (wherein Type I is defined as a structure which exhibits a flat or smoothly increasing type force displacement curve, while Type II exhibits a drop, or region of negative stiffness, in the force displacement curve) [96]. Type II structures are more sensitive to rate effects and are characterized by a drop in the force displacement curve after an initial peak - behavior which can be seen (albeit weakly) in the initial quasi-static loading cycle of the SC lattice in Fig. 4.2. This sharp drop arises due to the presence of buckling inducing a brief negative stiffness regime. Although wave localization can be seen in the strain data for all dynamic cases tested herein, in most cases the primary effect is the onset of layers deforming progressively from the site of impact in qualitatively the same manner as they do in the quasi-static case (albeit with some rate sensitive material behavior and relatively small inertia effects likely present). It is only in the Type II (SC) lattice that we can see this wave localization result in a qualitatively different deformation mechanism within a unit cell.

4.5 Conclusion

We have explored the mid-strain rate regime of soft polymer structures produced via AM, in the context of examining the shifting of the engaged deformation mechanisms as a function of strain rate and structure. We have shown that even at the lowest dynamic strain rate tested, there are indications in the strain data that a wave dominated regime, in which inertial effects matter, has been reached. This is despite similar studies in architected materials composed of metal that have often found that only constituent material strain effects exist at similar strain rates. We tie this to the effective wavelength in the material, which depends on the effective speed of sound - a parameter which, crucially, relies directly upon both the material and structure in question. This relationship can be expressed as a dimensionless localization parameter, $\frac{c\epsilon}{\dot{\epsilon}L}$, which indicates that a wave dominated regime has been entered when it is below unity. This parameter can be used as a judgment of the type of deformation regime a particular structure/material, at a particular

loading rate, can be expected to experience, which informs the most important mechanisms to be engaged. We summarize these differing regimes, as a function of $\frac{c\epsilon}{\dot{\epsilon}L}$, in Fig. 8.

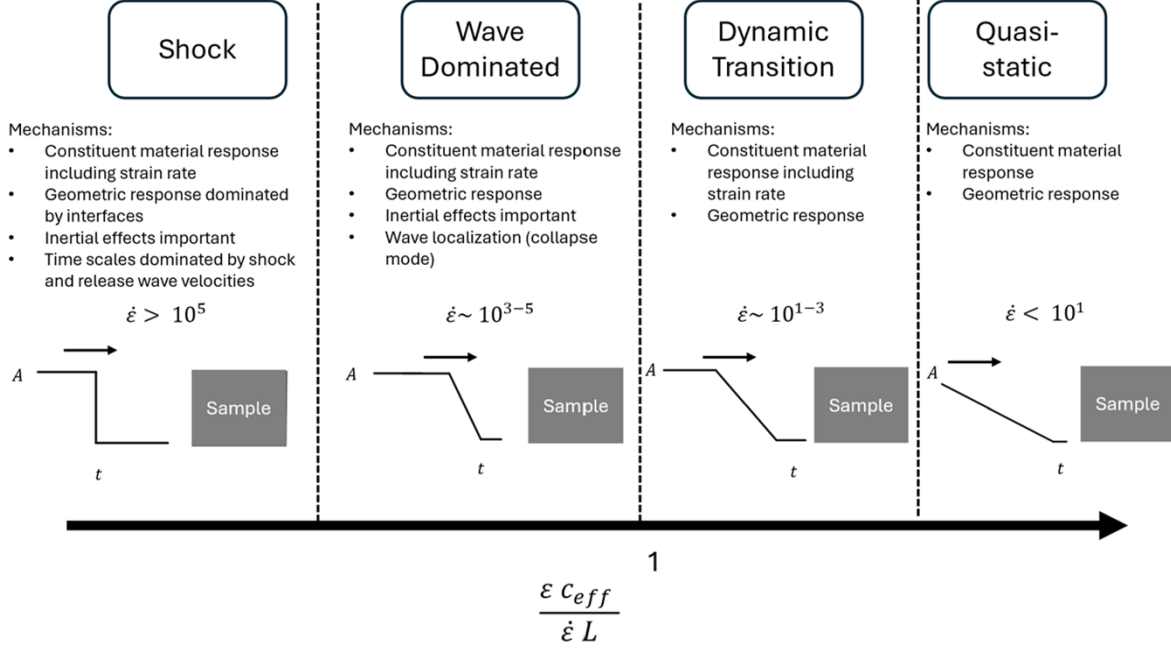


Figure 4.8. Regime map, outlining the regions in which qualitatively different mechanisms of deformation and energy absorption emerge as a function of the dimensionless parameter described in Equation 4.3. A shift to a wave dominated regime occurs below a value of 1.

Based upon these insights, we furthermore suggest the following broad design principles for AM lattice structures under dynamic loading. First, that the influence of the constituent material (namely upon ductility, stiffness, and sound speed), structure, and loading conditions ought to be considered when estimating if a wave dominated regime may be entered. When considering a wave dominated regime, the rate sensitivity of the geometry should be considered important in addition to the rate sensitivity of the constituent material. The type of structure should at this point gain further importance, keeping in mind that Type II structures tend to experience an effective strengthening due to inertial stabilization and dynamic buckling. This dynamic buckling can also be expected to induce a change in the mode of deformation within individual unit cells. Type I structures, meanwhile, may experience successive layer collapse in wave dominated regimes, but are less likely to display intra-cell deformation mode changes. We

further suggest that, in making these considerations, it may be helpful to consider the overall strain rate sensitivity as an effective ‘material’ property, wherein the effective material encompasses both structural and material influences upon the strain rate sensitivity. The localization parameter outlined herein can thus serve as a good rough guide as to expected regime, and therefore the anticipated importance of various mechanisms, which in turn can inform design and tailoring attempts. However, further examination of the space, including higher strain rates and different topologies, would be beneficial in refining estimates and fleshing out the design space.

4.6 Supplementary Information

Lattice Characterization

Here we include further information regarding the characterization of the additively manufactured lattices, including close up images (Fig. 4.9, bulk sample compression data (Fig. 4.10, and the effective elasticity modulus fits whose values are reported in Table 4.1 in the main text (Fig. 4.11).

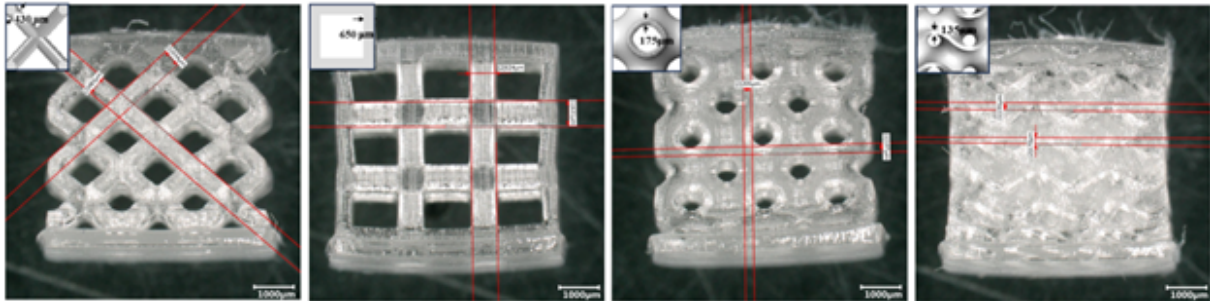


Figure 4.9. Close up images of the four lattice structure types. From left to right: BC, SC, P, G.

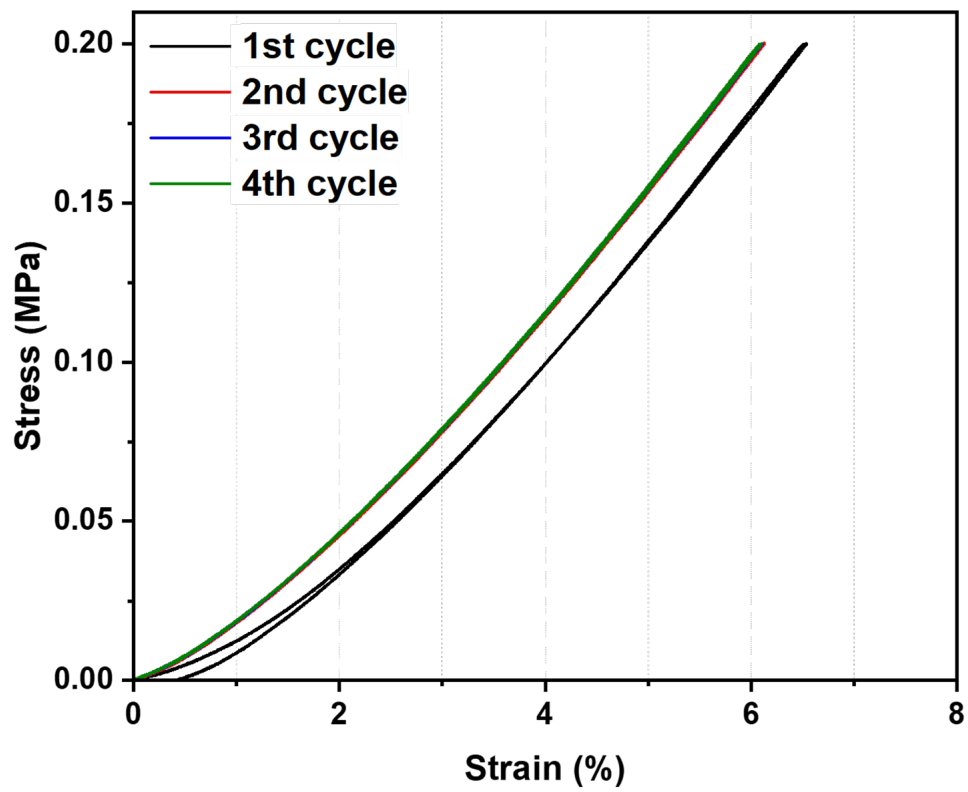


Figure 4.10. Bulk sample compression data

Processed Sensor Data

Figures 4.12-4.19 below show the strain and strain rate data taken from the incident bar strain gauge, for all samples tested at all input pressures.

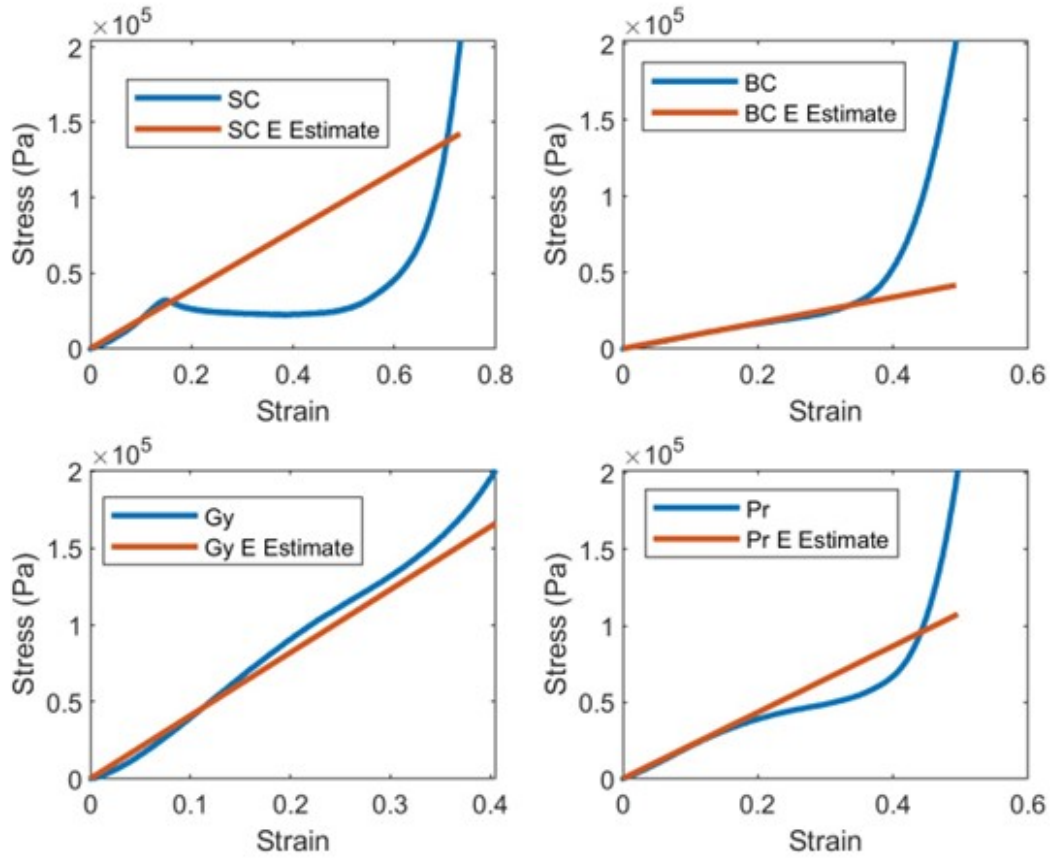


Figure 4.11. Linear fits used to calculate effective elasticity modulus, as reported in Table 4.1 in the main text. Fits were taken up to $\epsilon \sim 10\%$.

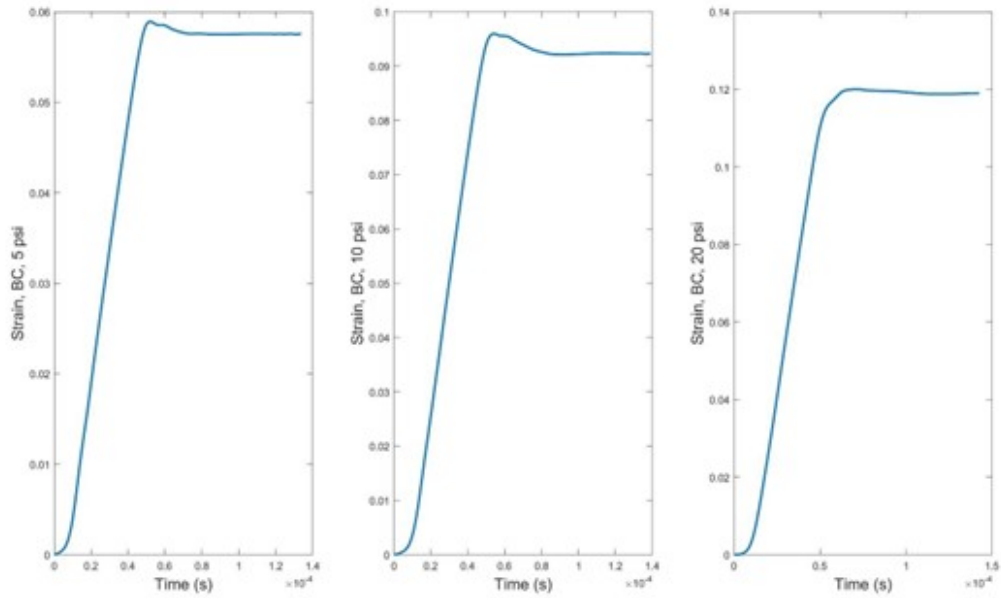


Figure 4.12. Incident pulse strain data taken from the incident bar strain gauge. Shown is the data for the BC samples at 5 psi, 10 psi, and 20 psi (from left to right).

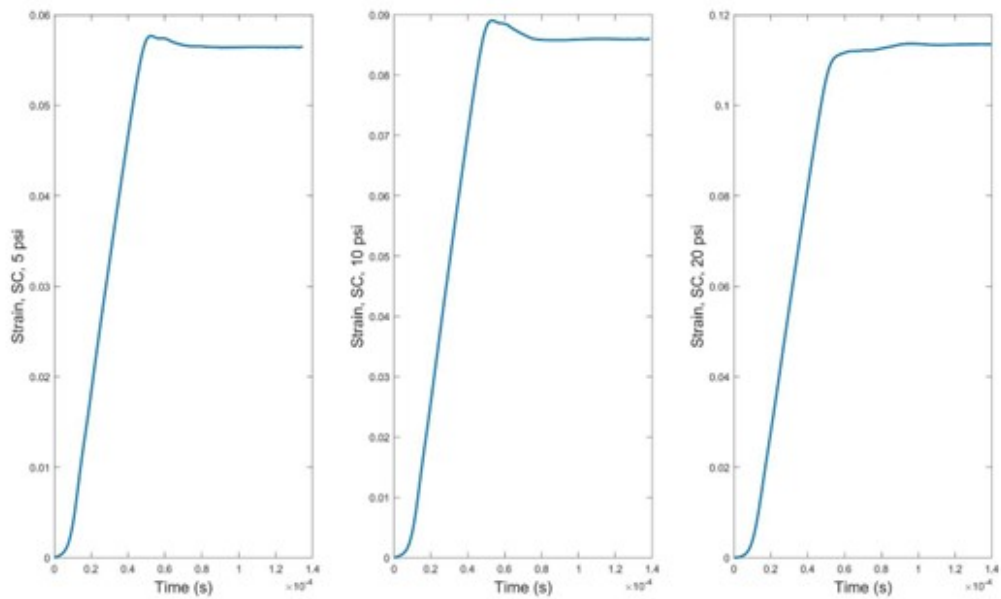


Figure 4.13. Incident pulse strain data taken from the incident bar strain gauge. Shown is the data for the SC samples at 5 psi, 10 psi, and 20 psi (from left to right).

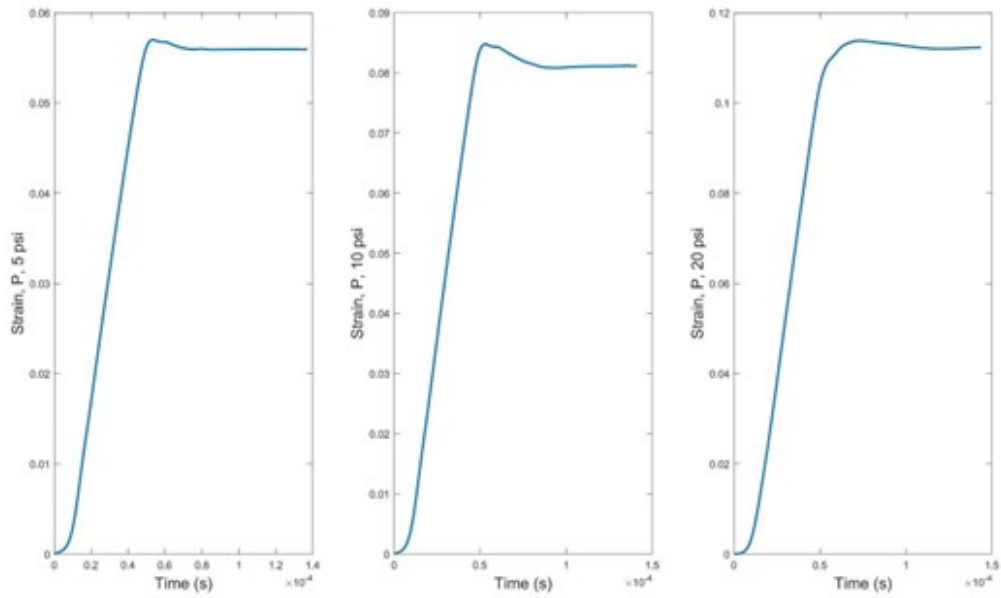


Figure 4.14. Incident pulse strain data taken from the incident bar strain gauge. Shown is the data for the P samples at 5 psi, 10 psi, and 20 psi (from left to right).

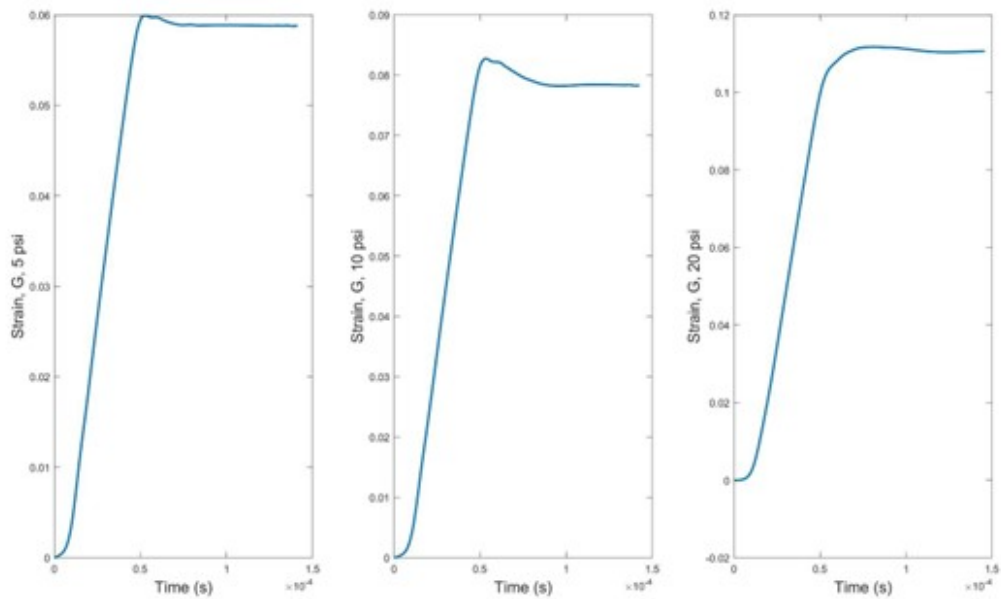


Figure 4.15. Incident pulse strain data taken from the incident bar strain gauge. Shown is the data for the G samples at 5 psi, 10 psi, and 20 psi (from left to right).

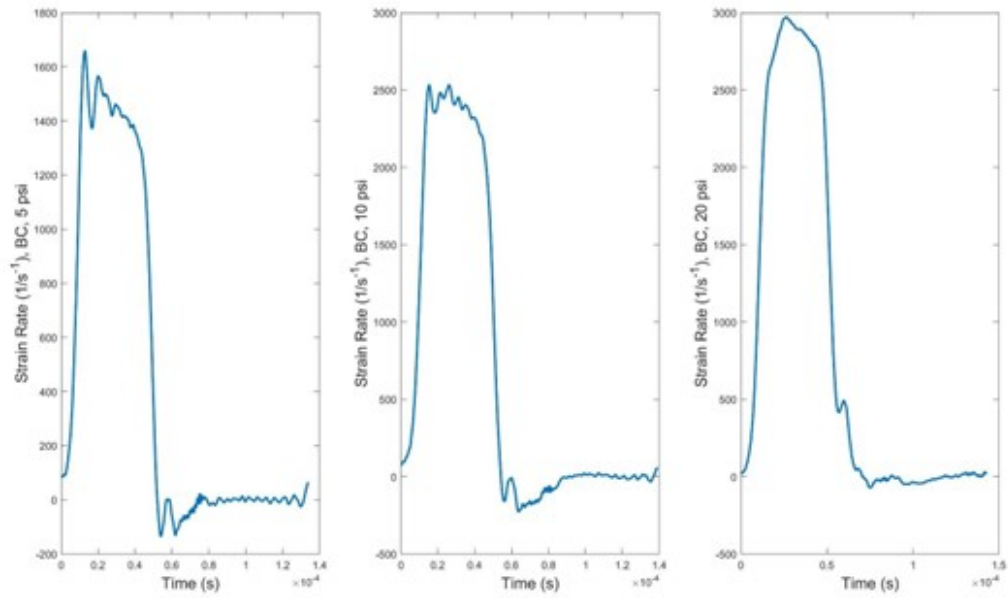


Figure 4.16. Incident pulse strain rate data taken from the incident bar strain gauge. Shown is the data for the BC samples at 5 psi, 10 psi, and 20 psi (from left to right).

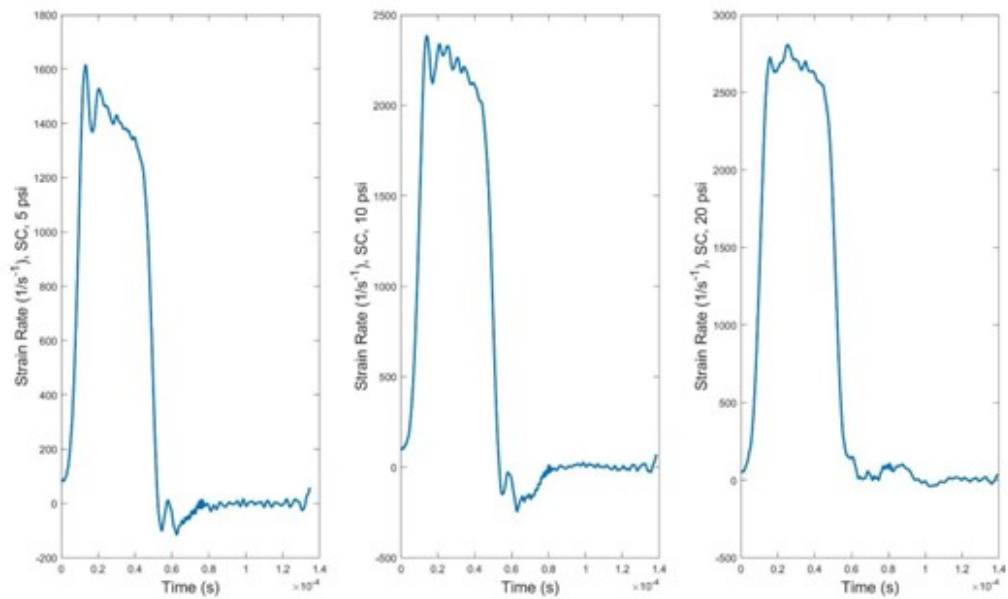


Figure 4.17. Incident pulse strain rate data taken from the incident bar strain gauge. Shown is the data for the SC samples at 5 psi, 10 psi, and 20 psi (from left to right).

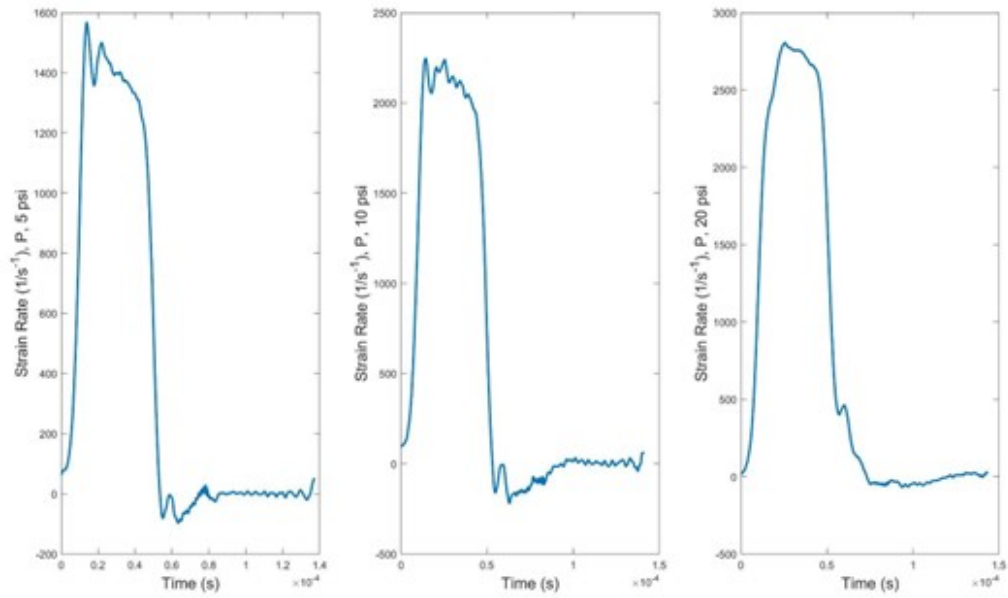


Figure 4.18. Incident pulse strain rate data taken from the incident bar strain gauge. Shown is the data for the P samples at 5 psi, 10 psi, and 20 psi (from left to right).

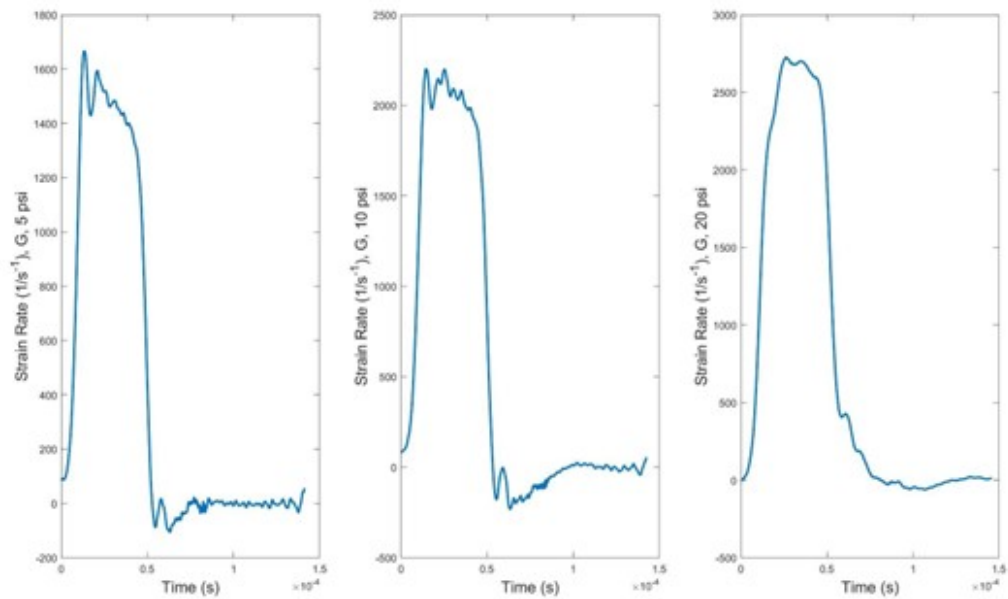


Figure 4.19. Incident pulse strain rate data taken from the incident bar strain gauge. Shown is the data for the G samples at 5 psi, 10 psi, and 20 psi (from left to right).

Processed DIC Data

Here we show further processed DIC data, beyond the selection shown in the main text. Included in the Figures 4.20-4.23 below are the vertically summed strain plots, with the data calculated as described in the main text. Data is shown here for each structure and test pressure. These plots encompass all times in the initial compressive pulse.

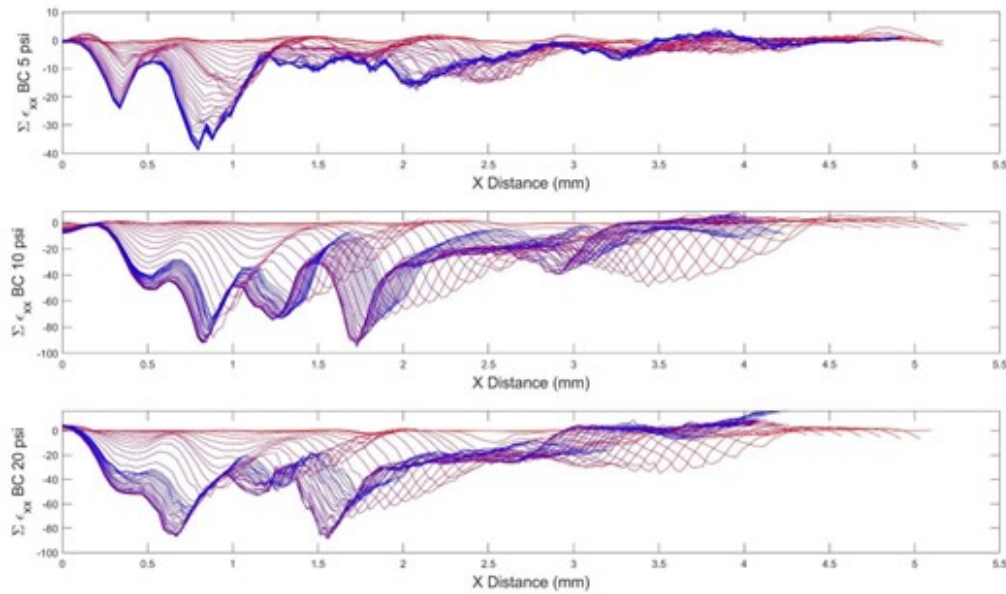


Figure 4.20. The vertically summed strain plots for the BC structure tested at 5, 10, and 20 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

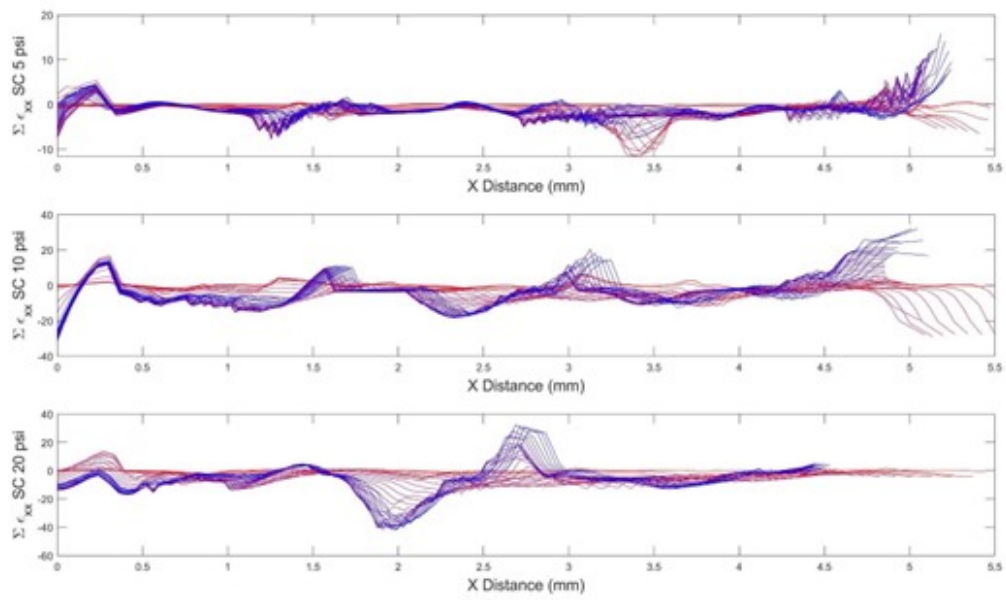


Figure 4.21. The vertically summed strain plots for the SC structure tested at 5, 10, and 20 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

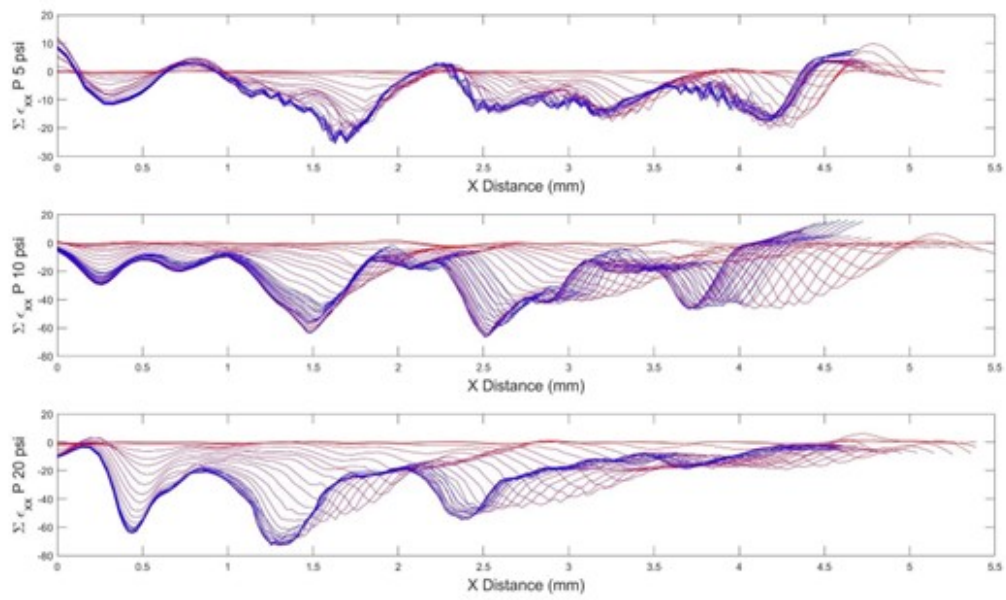


Figure 4.22. The vertically summed strain plots for the P structure tested at 5, 10, and 20 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

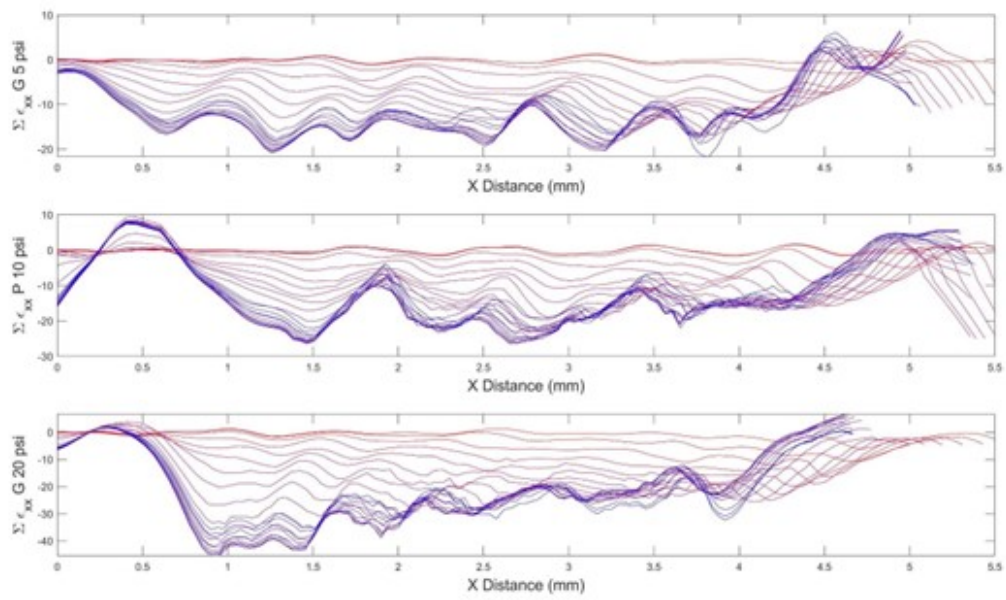


Figure 4.23. The vertically summed strain plots for the G structure tested at 5, 10, and 20 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

Figures 4.24-4.26 show the vertically summed strain plots, isolated for early time steps in order to highlight the localization of the deformation at the right (impact) edge, and the wave-like transition of the initial strain pulse across the length of the sample. The 5 psi input pressure cases in Figure 4.24 are also shown in the main text, and Figures 4.25-4.26 additionally include data for the input pressures 10 psi and 20 psi.

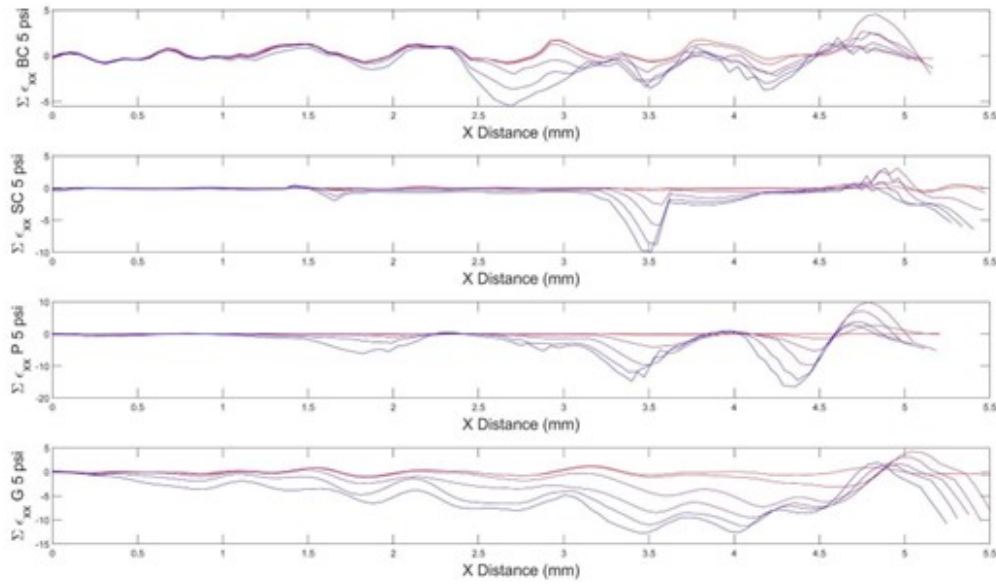


Figure 4.24. The isolated early time steps of the vertically summed strain plots for each structure at a test pressure of 5 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Plotted are the first five frames from the frame in which impact occurs. Time increases from red to blue, such that frame one is plotted as a red line and frame five is plotted as a blue line.

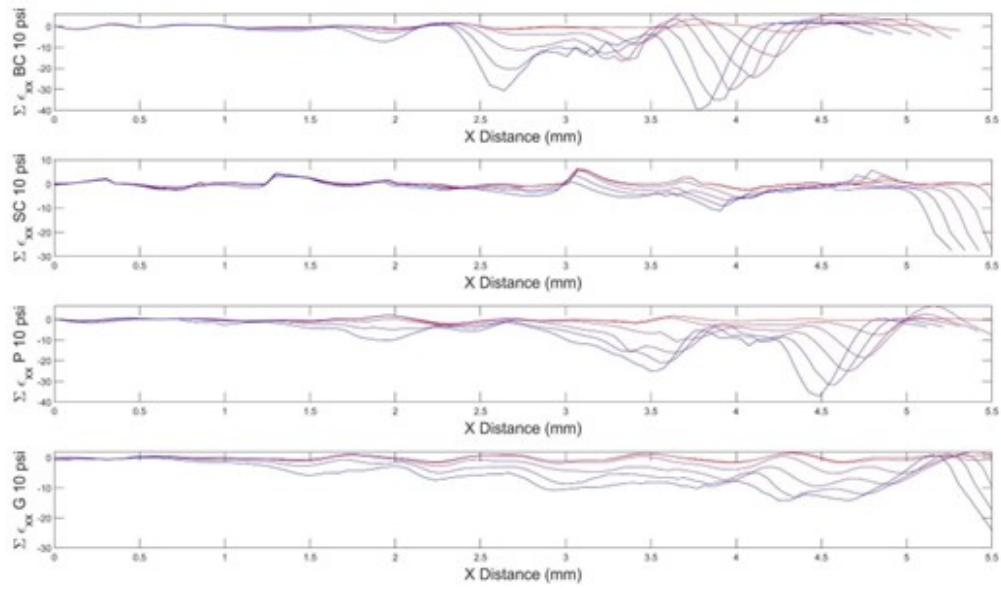


Figure 4.25. The isolated early time steps of the vertically summed strain plots for each structure at a test pressure of 10 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Plotted are the first five frames from the frame in which impact occurs. Time increases from red to blue, such that frame one is plotted as a red line and frame five is plotted as a blue line.

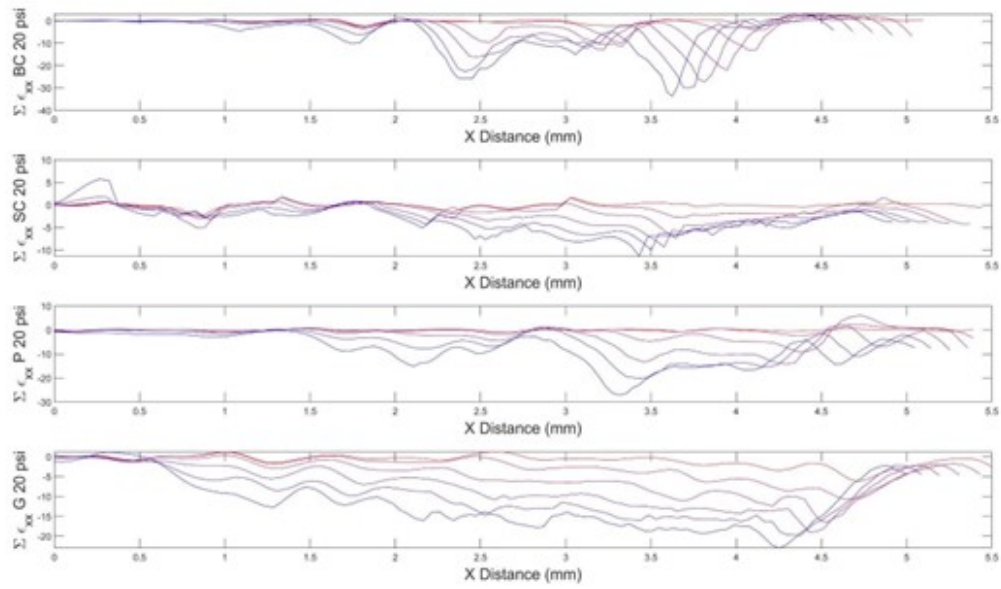


Figure 4.26. The isolated early time steps of the vertically summed strain plots for each structure at a test pressure of 20 psi, plotted with current (deformed) coordinates (the same as the examples currently in the main text). Plotted are the first five frames from the frame in which impact occurs. Time increases from red to blue, such that frame one is plotted as a red line and frame five is plotted as a blue line.

Included below in Figures 4.27-4.30 are plots of the same vertically summed strain measure as above and in the main text, but plotted with the reference (undeformed) coordinates rather than the deformed coordinates. This allows us to better see how much of the strain shifting is due to the sample itself being compressed (when using deformed coordinates, everything shifts to the left due to global sample compression), and how much is due to deformation localizing at different features on the sample.

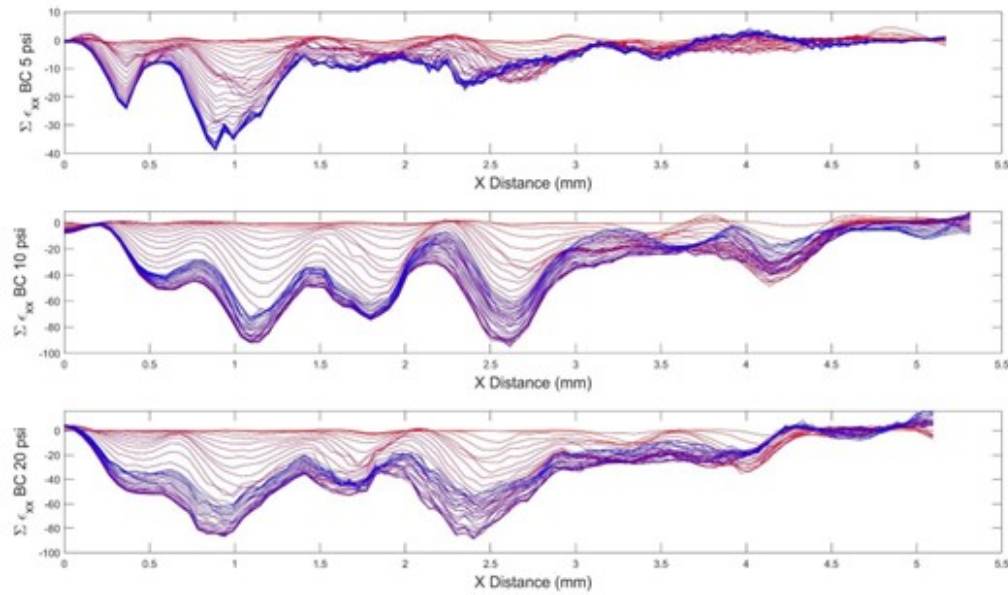


Figure 4.27. The vertically summed strain plots for the BC structure at test pressures of 5, 10, and 20 psi, plotted with reference (undeformed) coordinates. Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

4.7 Acknowledgements

Chapter 4, in full, is being prepared for submission. The dissertation author was the primary investigator and author of this material. Brianna MacNider, Dana M. Dattelbaum, Nicholas Boechler, Carl Cady, Benjamin K. Derby, Saryu Fensin, Kwan-Soo Lee, Jihyeon Kim, Nitin Daphalapurkar, Sushan Nakarmi.

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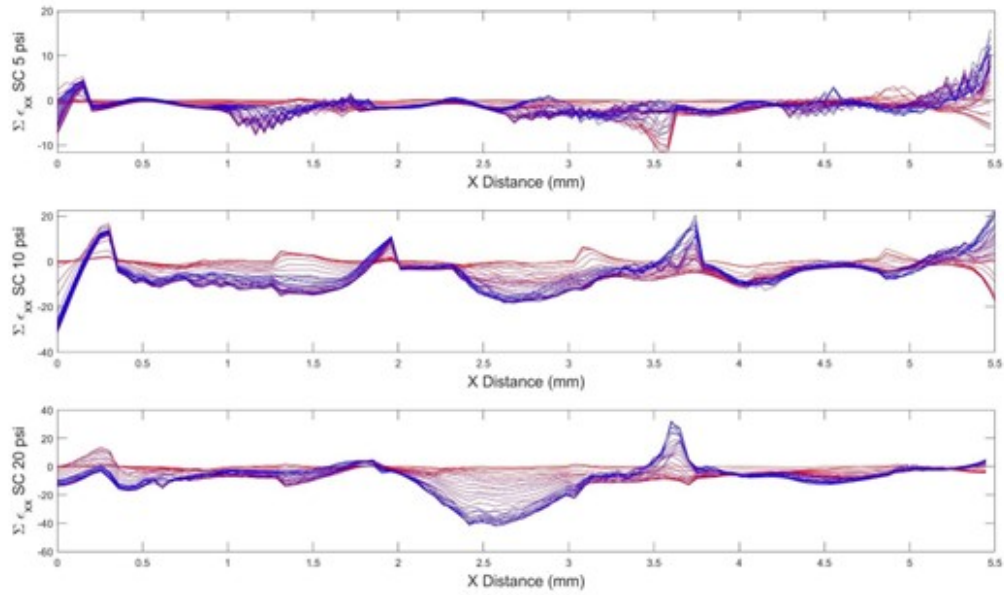


Figure 4.28. The vertically summed strain plots for the SC structure at test pressures of 5, 10, and 20 psi, plotted with reference (undeformed) coordinates. Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

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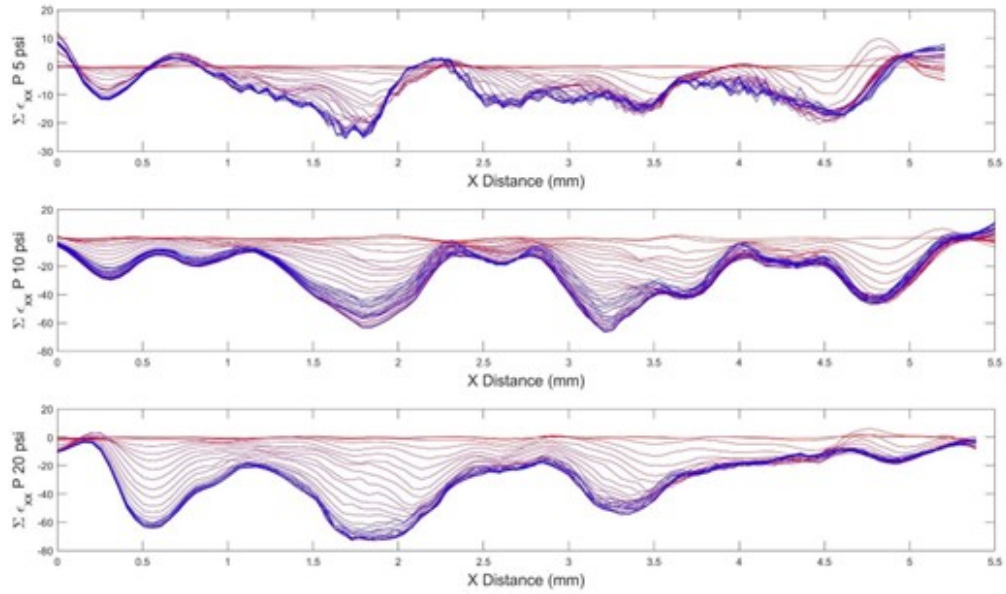


Figure 4.29. The vertically summed strain plots for the P structure at test pressures of 5, 10, and 20 psi, plotted with reference (undeformed) coordinates. Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

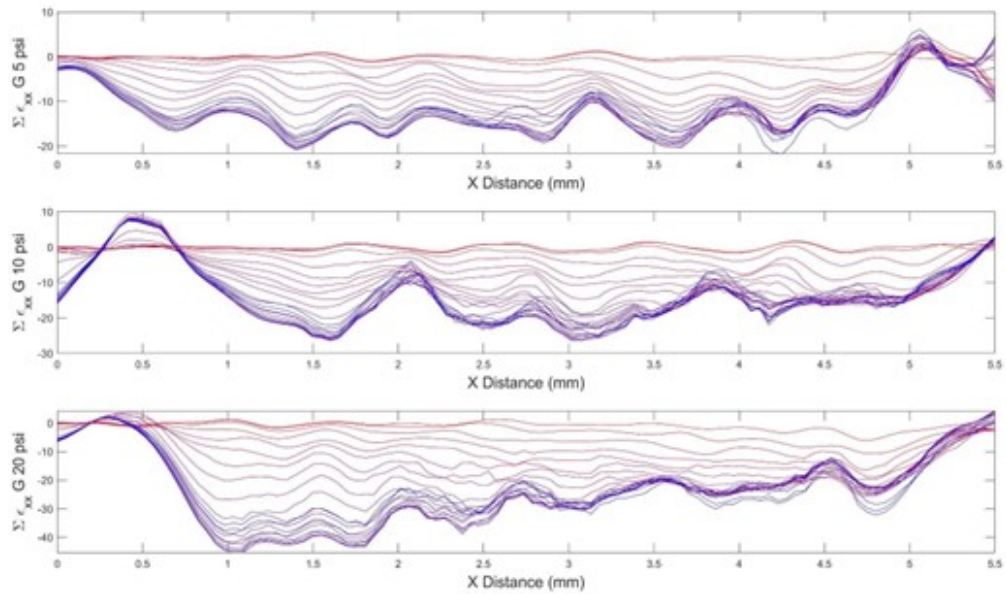


Figure 4.30. The vertically summed strain plots for the G structure at test pressures of 5, 10, and 20 psi, plotted with reference (undeformed) coordinates. Time increases from red to blue, such that early times are plotted as red lines and late times are plotted as blue lines.

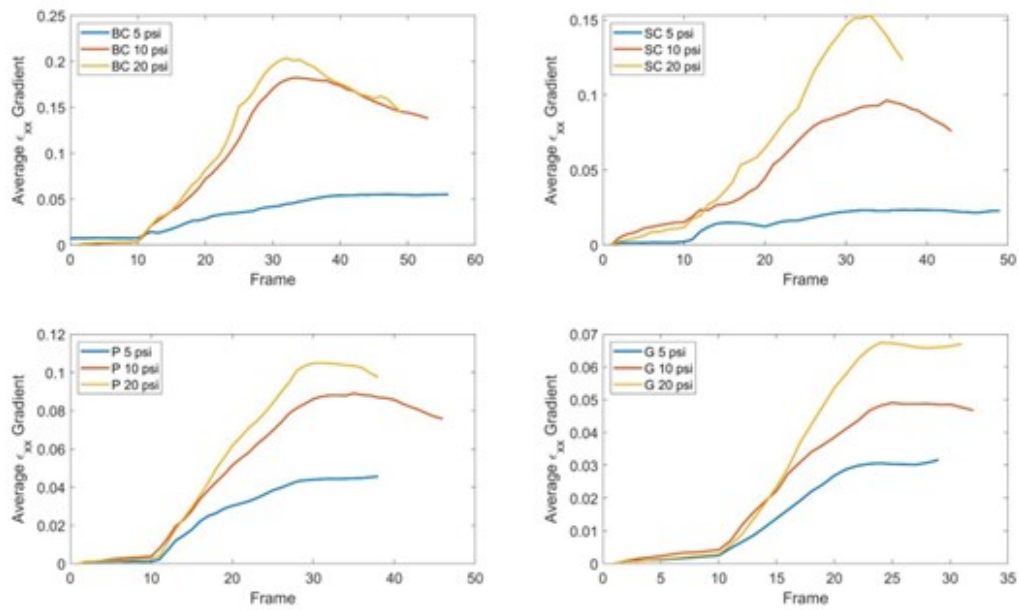


Figure 4.31. Averaged gradient of the x strain field, in which the absolute value of x strain gradients were averaged over each entire frame. Note the y-axis scale differences between these plots. BC has the highest strain gradient values, followed by SC, P (although P is close to SC), and finally G.

Chapter 5

In situ measurement of damage evolution in shocked magnesium as a function of microstructure

Accurate modeling and prediction of damage induced by dynamic loading in materials has long proved to be a difficult task. Examination of post-mortem recovered samples cannot capture the time-dependent evolution of void nucleation and growth, and attempts at analytical models are hindered by the necessity to make simplifying assumptions, due to the lack of high resolution, in-situ, time-resolved experimental data. Here, we use absorption contrast imaging to directly image the time evolution of spall damage in metals at $\sim 1.6 \mu\text{m}$ spatial resolution. We observe a dependence of void distribution and size on time and microstructure. The insights gained from this data can be used to validate and improve dynamic damage prediction models, which has the potential to lead to the design of superior damage resistant materials.

5.1 Introduction

Predicting nucleation and growth of void damage in ductile metals under dynamic loading remains a challenging problem to which much effort has been devoted [113, 126, 127, 220–222]. Under shock and subsequent release loading, it is well known that the interaction of the resulting rarefaction waves can lead to the creation of a region of transient tensile stress, eventually inducing nucleation of voids at defects in the microstructure. This phenomenon, known as

spall [123, 124], eventually leads to material failure as nucleated voids grow and coalesce. It is therefore of interest to investigate void formation and evolution within the context of the development of more robust damage resistant materials [223].

To model and predict the overall dynamic failure process, it is important to have a quantitative understanding of the contributions and evolution of the underlying mechanisms. Extensive experiments and simulations have been performed to investigate the effects of relevant parameters on spall strength. It has been found that loading conditions [224–226], crystal orientation [128, 227–229], structure [230, 231], grain boundaries [232–236], defects [237, 238], and anisotropy [239] have an effect on material behavior and void damage evolution under spall loading. Many analytical void damage models have been developed which attempt to predict spall strength and void evolution over time [222, 240]. Models have incorporated effects such as void nucleation and growth [241], rate dependency [242, 243], and void coalescence [244], to name a few, with varied degrees of success in predicting experimental data.

We suggest that insufficient understanding of void nucleation and growth is a critical barrier to accurately predicting void-driven damage, and thereafter, ultimate failure in ductile materials. While molecular dynamics (MD) simulations have been used to capture many features of spall experiments at high strain rates (e.g. Ref. [245]), they have shown substantial discrepancies at lower strain rates, due to limits on system size and computation time [246, 247]. This is particularly relevant to the gas gun impact experiments shown herein (with strain rates $\leq 10^5 \text{ s}^{-1}$), and is important because it has been shown that strain rate has a notable effect on total damage in materials [248]. Deficiencies in current analytical strain-equivalent damage models [222, 240–242, 244] for nucleation and growth include assumptions and simplifications of the initial positioning of void nucleation sites, void growth rates, and void shapes. This lack of understanding is, in part, related to the absence of direct, real-time quantitative measurements of void nucleation and early-stage growth. Such in-situ observations had, until recently [249–252], remained a grand experimental challenge, largely due to the extremely fine spatial (μm) and, simultaneously narrow (ps) and extended (μs) temporal, scales involved in shock-induced spall

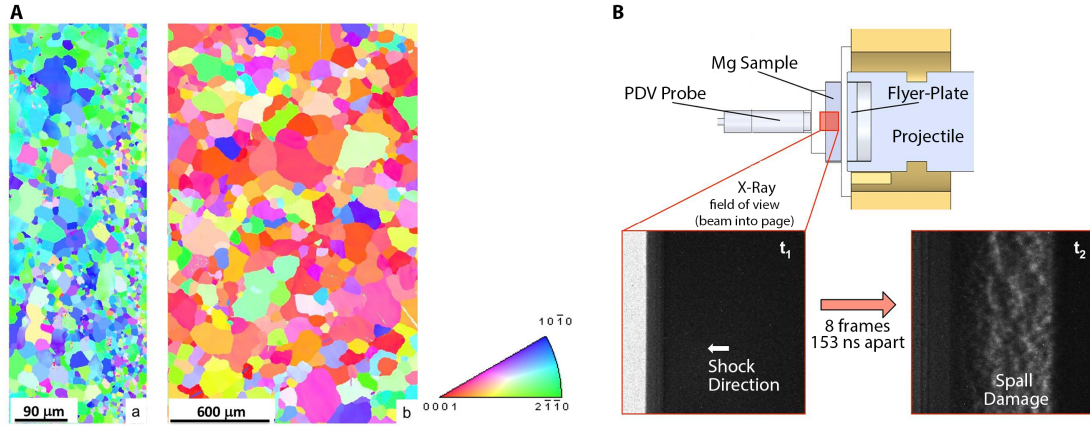


Figure 5.1. Polycrystal characterization and experimental setup. (A) Inverse pole figure maps, obtained from electron backscatter diffraction measurements, of the pre-deformation AZ31B (left), and pure magnesium (right) polycrystalline samples in the through-thickness direction. Reused from Ref. [253] with permission of author. (B) Diagram of the plate-impact experiment setup, with detail on the right demonstrating the x-ray field of view, as well as the impact and shock directions. The magnesium sample was held in a lexan mount, affixed to a brass ring that allowed the sample to be aligned normal to the gun barrel. The PDV probe was mounted a few mm from the rear of the sample.

experiments. In recent years, studies using post-mortem measurements [124, 224–226, 236] have well established that under dynamic loading conditions, microstructural features such as grain boundaries, inclusions, vacancies and heterogeneities can preferentially act as void nucleation sites. Even though there has been some progress in predicting void nucleation at various microstructural features [128, 227, 228], void growth and evolution modeling remain a challenge. Single post-mortem images lack insight into time-dependent processes, and no real-world, time-resolved data exists regarding void growth in ductile metals.

In this work, we present in-situ, time-resolved, high-resolution measurements of early-stage void growth in ductile metals experiencing spall under shock loading. This new data proposes to fill a gap in our understanding of dynamic damage evolution and inform current

void damage models, as well as lead to the development of new ones. We focus on high-fidelity ($\sim 1.6 \mu\text{m}$ spatial resolution) void distribution data in magnesium, which was chosen as a model material due to interest in the effects of its high anisotropy. In addition, substantial interest has been shown in its behavior under spall conditions [126], and its low absorption length for a metal makes it especially suitable for experiments at the x-ray energies and flux available at the Dynamic Compression Sector (DCS). While radiography data has been utilized to investigate dynamic fracture and crack propagation previously [249, 251, 252, 254], these experiments have not been used to investigate spall-driven void evolution in metals. Still other attempts at investigating spallation in metals have utilized proton radiography [255], but, crucially, this approach is limited in the achievable spatial resolution (maximum of $60 \mu\text{m}$ [256]), restricting this previous analysis to the scale of spall layers ($\sim 0.6 - 1 \text{ mm}$) rather than nucleation and growth on the level of individual voids. Some work has been done in utilizing x-ray diffraction to investigate time-resolved spallation in metals [257], but this data crucially lacks direct measurements of void distribution, shape, and growth. Our measurements of spallation in magnesium as a function of varying microstructure demonstrate the dependence of damage evolution upon microstructure and loading direction, highlighting a divergence from the simplifying assumptions often made in predictive models. We furthermore show that spall strength alone is not a good indicator of how void damage will evolve, underscoring the importance of these type of high-resolution in-situ measurements in order to obtain a complete picture of material behavior during spallation. This data provides critical insights into a regime which has, up until now, been characterized by approximations.

5.2 Results

Flyer-plate driven incipient spall experiments were performed on three varieties of magnesium to systematically determine the affect of microstructure and chemistry on spall induced void damage and failure. The microstructural effects were captured by investigating

single crystal and polycrystalline pure Mg (99.99%). The effects of sample chemistry were sampled by including polycrystalline AZ31B Mg. Figure 5.1a shows electron backscatter diffraction analysis of the polycrystalline and AZ31B samples. It was found that AZ31B had grain sizes ranging from approximately $10\text{ }\mu\text{m}$ to $40\text{ }\mu\text{m}$, and the average grain size of the pure magnesium was approximately $100\text{ }\mu\text{m}$. X-ray absorption contrast imaging allowed the capture of a series of eight frames showing the evolution of the spallation process through the thickness of each sample, achieving a frame rate and spatial resolution of 153 ns and $1.6\text{ }\mu\text{m}$, respectively. We note that, while this spatial scale does not enable the discernment of sub-micrometer void nucleation sites, it allows the characterization of micrometer-scale voids. In general, voids nucleate, coalesce, and grow throughout the damage process. Because of our resolution limit, the voids we measure at a given time are a subset of this greater population. As the damage process evolves in time, we expect that previously unmeasured voids add themselves to the measured population via coalescence and growth. Post-processing and normalization of the x-ray images is discussed in the Methods section. A schematic of the experiment and diagnostics is shown in Figure 5.1b.

Examination of the x-ray imaging data provides an in-situ view of void evolution as a function of time, which provides insights into the evolution of void distribution and the effects of crystal orientation and chemistry on the evolution of void damage in metals. A complete set of frames from a single dynamic experiment on polycrystalline Mg impacted at $0.39\text{ mm }\mu\text{s}^{-1}$ is shown in Figure 5.2 as a representative set of the type of data collected for all samples. The higher intensity red and white regions in this figure represent areas of low density (free surface or voids). An evolution can clearly be seen not only of the width of the spall plane, but also of its morphology. We note that it is possible for intensity distribution to be affected by changes in the tilt of the sample during impact, thus, a combination of image analysis of the rear free surface and previous photon doppler velocimetry (PDV) velocity-time data from a similar system was used to estimate an expected tilt of 1-2 mrad (see SI). This work therefore assumes that any changes in the intensity are associated solely with changes in void number and size.

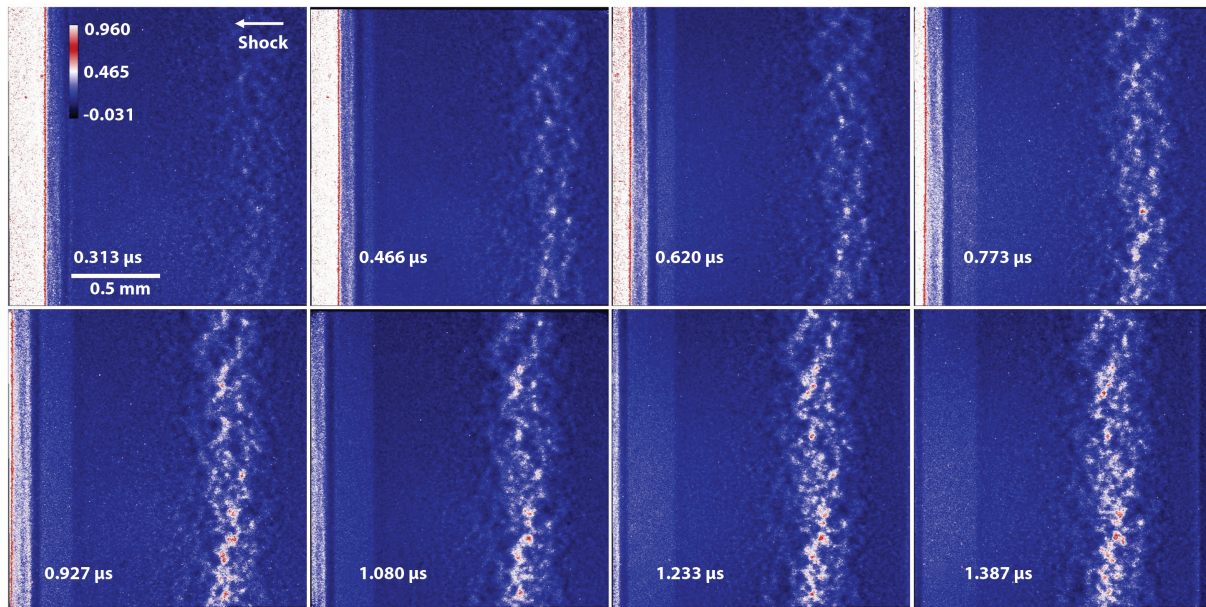


Figure 5.2. Time evolution of spall-induced void formation in polycrystalline magnesium. X-ray images for polycrystalline magnesium, at an impact speed of $0.39 \text{ mm } \mu\text{s}^{-1}$, with the shock traveling from right to left. Times with respect to impact (time zero) are included on each image. The scale bars in the top left frame show intensity (arbitrary units) and length scales, and apply to all frames in this figure. Additional color adjustments have been performed for visibility, in which red represents the highest intensity (least dense, free surface and strongest voids), blue the lowest intensity (most dense, target), and white in between (majority of voids).

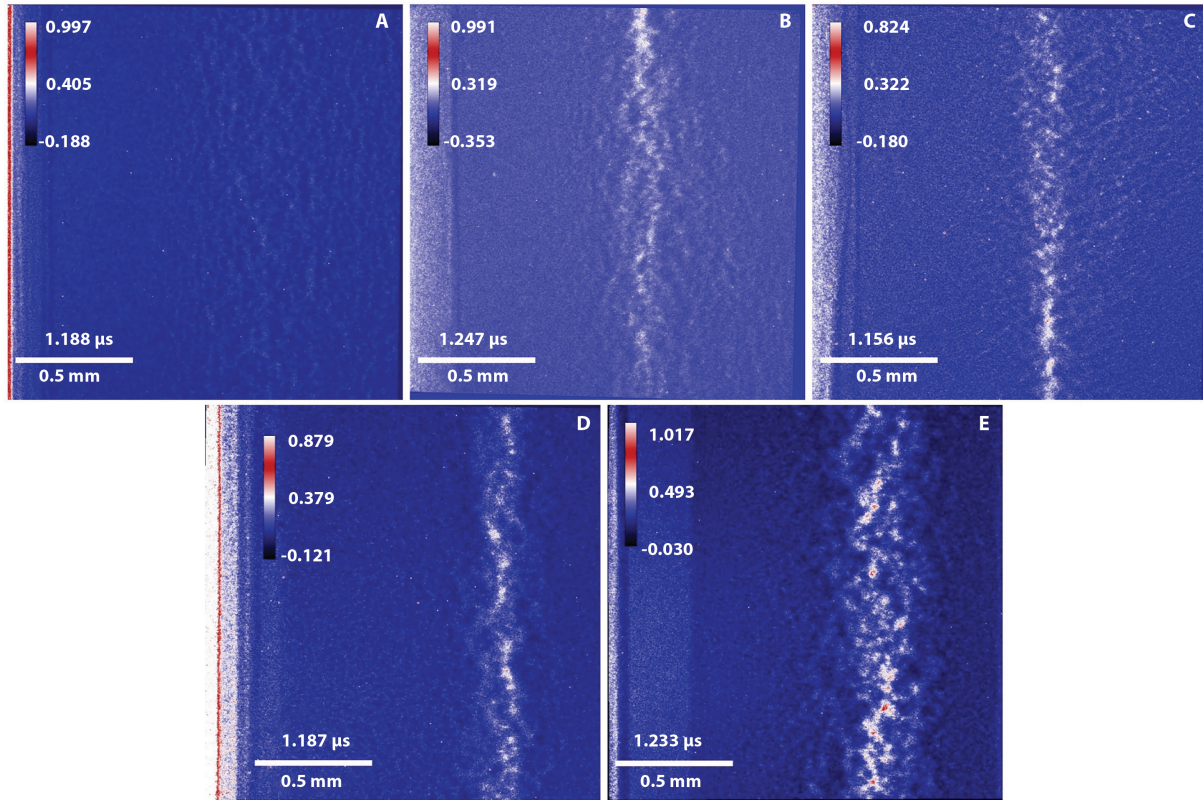


Figure 5.3. A comparison of void damage in x-ray images from varying samples at similar times. (A) single crystal $[0001]$, (B) single crystal $[11\bar{2}0]$, (C) single crystal $[1\bar{1}00]$, (D) AZ31-B and (E) pure polycrystalline magnesium. Impact speed for all samples shown was $0.4\text{ mm}\mu\text{s}^{-1}$. Note that additional color and brightness adjustments have been performed for visibility in these images to make void shapes more visible (as noted by the inconsistent intensity scales [arbitrary but proportional units]).

In general, microstructure, as defined by chemistry and orientation, is known to substantially affect void nucleation and growth under shock loading [128, 228, 258], as well as spall strength and morphology of the damage plane [231]. Figure 5.3 shows x-ray images of different Mg samples, impacted at the same velocity, at approximately the same time with respect to impact. We note that additional brightness adjustments have been performed on these images in order to more easily identify void characteristics. Images without brightness adjustment and with the same intensity range have been included in the SI, and a more thorough quantitative examination of accumulated void damage without brightness adjustments is examined later in our results. Through qualitative examination, we see that there is a marked difference in void shape and distribution between the various microstructures. The top panel in Figure 5.3 compares results as a function of orientation in single crystal Mg, and highlights variations in the total amount and morphology of the void distribution. In particular, it is of note that the x-ray images corresponding to the $[0001]$ orientation show a low porosity, implying a high resistance to spall damage (Figure 5.3a). Additionally, there are clearly differing shape and preferential growth directions of the void damage plane in the $[11\bar{2}0]$ (Figure 5.3b) and the $[1\bar{1}00]$ orientations (Figure 5.3c). Both the $[11\bar{2}0]$ and $[10\bar{1}0]$ orientations show long, thin extensions of void damage away from the spall plane, in line with observations in molecular dynamics (MD) simulations in [259], which note the nucleation of voids at planar stacking fault interactions, and the non-spherical nature of the resulting voids. In addition, MD investigations performed in [238] identify that void shape and growth is dominated by different mechanisms depending on the crystal orientation, noting the domination of $\{11\bar{2}2\}\{11\bar{2}3\}$ pyramidal dislocations and twinning in the $[0001]$ orientation, and the domination of $\{1\bar{1}00\}\{11\bar{2}0\}$ prismatic dislocations, and a lack of twinning, in the $[10\bar{1}0]$ case, as well as the presence of non-spherical voids in both single crystal orientations. While we note that previous MD work cannot be compared quantitatively with the experimental work herein due to inherent differences in model assumptions, nonetheless it can provide valuable information concerning trends and insight into mechanisms.

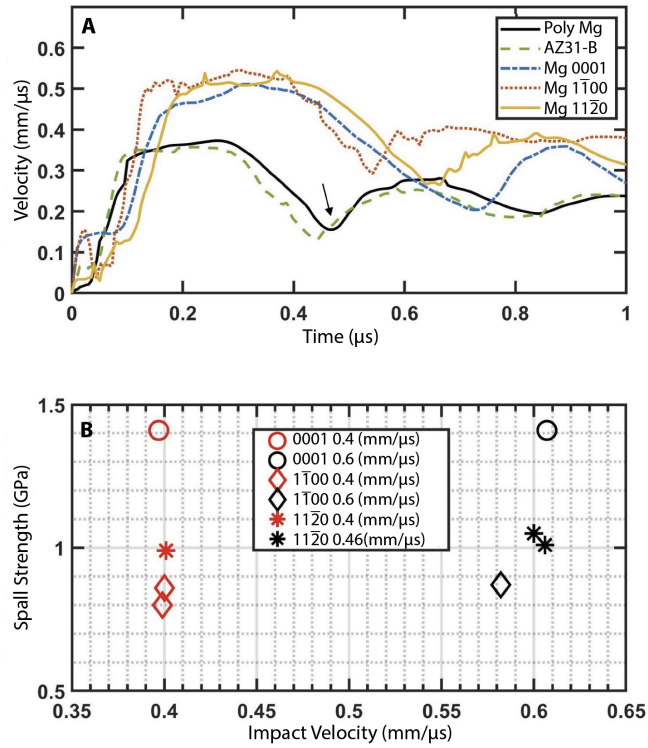


Figure 5.4. PDV and single crystal spall strength data. (A) PDV velocity data for single crystal [0001], single crystal [11 $\bar{2}$ 0], single crystal [1 $\bar{1}$ 00], AZ31-B, and pure magnesium. Impact speed for all samples shown was 0.4 mm/ μ s⁻¹. The arrow demonstrates the pull-back minima for a single data set (polycrystalline Mg). (B) Calculated spall strength values for all single crystal experiments, including multiple impact velocities.

The x-ray imaging results were compared to spall strength, calculated from the time-velocity history, and found to be qualitatively consistent with the observed damage accumulation, as the [0001] orientation was found to have both the highest spall strength and the highest resistance to damage evolution (lowest observed voids), while the other orientations display lowered spall strength and a greater number of visible voids. The velocity-time for the different experiments is shown in Figure 5.4. Spall strength was calculated using

$$\sigma_{spall} \equiv \frac{1}{2} \rho_o C_B (\delta u_{fs}), \quad (5.1)$$

as found in the work of Kanel and Gluzman [133, 134], where ρ_o is the initial density, C_B is the measured bulk sound speed (measured herein using standard pulse echo method), and δu_{fs} is the difference in the free surface velocity from the peak state to the pull-back minima (see Figure 5.4).

Calculated spall strengths for the single crystals are shown in Figure 5.4 as a function of orientation and impact velocity, and the values of the other parameters relevant to the spall calculations for these experiments are included in the SI. Several experiments were repeated with similar conditions to test for repeatability (see the SI for more information). Of note, the [0001] orientation is shown to have by far the highest spall strength, consistent with the qualitative resistance to void formation and growth noted in the images in Figure 5.3.

The qualitative observations noted in Figure 5.3 were quantified in each case through the use of intensity averaging techniques, described in more detail in the Methods section. A compilation of vertically averaged intensity plots for the different microstructures at a similar impact velocity are shown in Figure 5.5, which examines intensity values that have been normalized relative to one another. Although we note that there may be lower scale damage that is not captured by the resolution of the technique, and that the through-thickness void damage has been compressed into a two-dimensional representation, the examination of void-induced intensity (corresponding to x-ray transmission) presented in this work can still provide valuable

insights into void distribution evolution and growth rates. This figure highlights differences in the width, shape, and growth rate of the relative intensity curves. In general, it can be seen that the total porosity increases with time, and that the void distribution begins to suggest a change from Gaussian to bimodal in some microstructures as a function of time, with the polycrystalline and AZ31B experiments showing a broadening of the damage peak and the emergence of bimodal damage distribution at intermediate times. In addition, as sample microstructures become complex due to the presence of grains of multiple orientations and varying chemistry, an increase in void damage as compared to the single crystals is observed. This is highlighted by an increase in peaks and widths of intensity in Figure 5.5 and markedly different morphology of the spall plane in Figures 5.3d and 5.3e. This observation is not unexpected, as the existence of a greater number of potential nucleation sites in the polycrystalline samples is expected to decrease spall strength and produce a greater number of voids in comparison to single crystals. Additionally, we note differences in the width and intensity of the spall plane amongst the polycrystalline (AZ31B and pure Mg) samples. In general, chemistry of the material, texture, grain size, and other microstructural features can affect spall. Due to the higher impurity content of AZ31B potentially providing more nucleation sites, it might be expected for pure Mg to have higher resistance to void nucleation. However, here, pure Mg is observed to have greater void damage. We hypothesize that the grain size is the dominant factor driving this, as the material characterization showed the polycrystalline Mg to have larger grains than AZ31B, and previous works have shown that materials with larger grain size tend to promote easier and higher amounts of void growth in comparison to materials with a smaller grain size [260]. This is qualitatively consistent with the data from the x-ray images. However, it is important to note that the varying chemistry between AZ31B and polycrystalline Mg may also be contributing by altering the deformation mechanisms during shock loading, affecting the number of void nucleation sites available.

In order to quantify the variations in the spall behavior, the intensity measurements shown in Figure 5.5 were integrated across the width of the spall plane, and this area was taken as

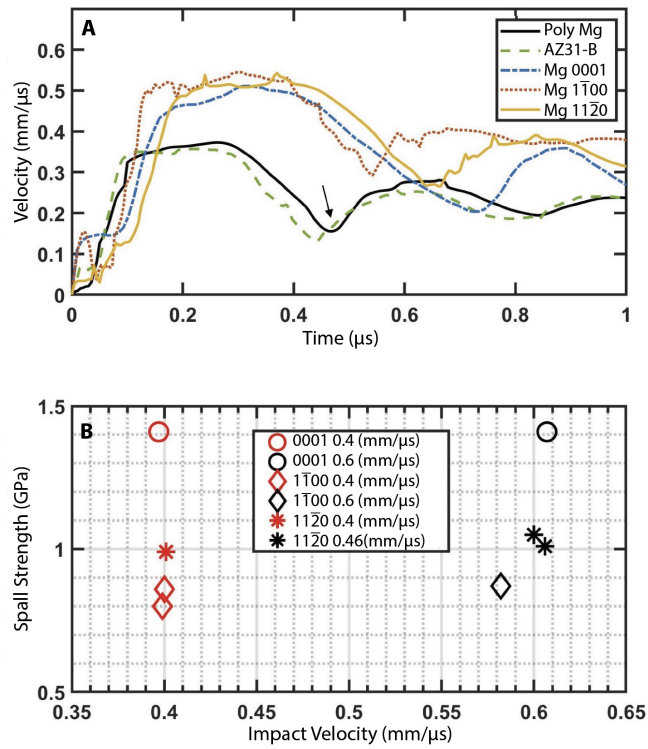


Figure 5.5. Comparison of averaged intensity across frames. Averaged intensity comparisons are shown for a single crystal in three orientations, AZ31B, and Pure Mg. The color represents the vertically averaged intensity value at each x-location.

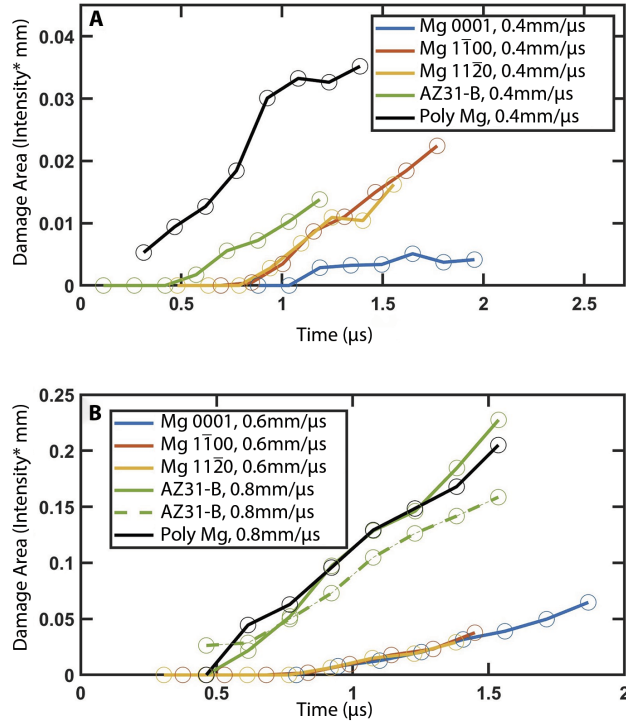


Figure 5.6. Comparison of integrated intensity across the width of the spall plane, representative of the transient integrated damage, for each material and at varying impact speeds. (A) Integrated intensity for an impact speed of $0.4 \text{ mm } \mu\text{s}^{-1}$, highlighting the substantial differences in accumulated damage between various microstructures at lower impact speeds. (B) Integrated intensity at higher impact speeds, including $0.6 \text{ mm } \mu\text{s}^{-1}$ (single crystal samples) and $0.8 \text{ mm } \mu\text{s}^{-1}$ (polycrystalline and AZ31B samples), highlighting the reduced (but still present) importance of microstructure as impact speed is increased.

the approximate accumulated void damage through the depth of the sample, at that time. It should be noted that this approach incorporates low intensity regions through the thickness of the sample, and is not an absolute measure of damage, but it does provide valuable insights when comparing relative void damage between experiments run with different samples and impact speeds. In Figure 5.6a, the areas were compared as a function of time from impact for different samples under the same loading conditions (an impactor velocity of $0.4 \text{ mm } \mu\text{s}^{-1}$). At this lower impact velocity, when accounting for both width of the spall plane and intensity, polycrystalline magnesium was shown to accumulate the highest amount of void damage. This is followed by AZ31B, single crystal $[1\bar{1}00]$ and $[11\bar{2}0]$, and finally the $[0001]$ samples. These results are consistent with the previous understanding regarding the role microstructure plays in determining void nucleation and growth, as well as our observations in Figure 5.5. When examining the spall strength of single crystal Mg, we do note a slight discrepancy in comparison to other results in literature - namely, that the $[0001]$ orientation is found by Kanel et al. [261] to have the lowest spall strength among the crystal orientations. Meanwhile, the high spall strength and drastically lowered void damage profile in the $[0001]$ orientation is very clear in our results. As spall strength can vary widely depending upon loading conditions, we hypothesize that the variation between our works in sample thicknesses, loading stresses, and peak strain-rates during experiments make a direct comparison of single crystal trends between the two works invalid. Additionally, at the comparatively low impact velocities used in this study ($0.4 \text{ mm } \mu\text{s}^{-1}$ - $0.6 \text{ mm } \mu\text{s}^{-1}$), there is some agreement with our observed spall strength trends in MD work [238].

As the impact velocity was increased, a shift in some of the porosity trends is observed, as seen in Figure 5.6b. For instance, the high void damage resistance in the $[0001]$ orientation reduces at the higher impact velocity of $0.6 \text{ mm } \mu\text{s}^{-1}$, bringing the damage amount in line with that in other orientations, although the spall strength remains high, as per Figure 5.4. This suggests that, while spall strength and void damage evolution are related, spall strength alone is not a complete descriptor for void formation and eventual failure in materials. Another key

observation is the altered void accumulation in AZ31B in comparison to pure Mg. For the $0.4 \text{ mm} \mu\text{s}^{-1}$ experiments, AZ31B showed substantially lower porosity than polycrystalline Mg, but at impact velocities of $0.8 \text{ mm} \mu\text{s}^{-1}$, their performance is comparable. Both trends are consistent with the understanding that as the impact velocity is increased above a critical value, microstructure plays less of a role in controlling damage and failure [260]. We hypothesize that the $0.6 \text{ mm} \mu\text{s}^{-1}$ and $0.8 \text{ mm} \mu\text{s}^{-1}$ impact speeds are in the region of this impact velocity, resulting in the reduced differences noted between disparate samples, and that at even higher impact velocities than those tested here, even less of a disparity would exist between the void damage curves of the single crystal and polycrystal Mg.

The rate of damage accumulation is an important parameter needed to calibrate void growth models and can now be estimated through examining the time-resolved data presented in this work. The slopes of the curves in Figure 5.6 were examined, allowing for an estimation of the rate at which this damage accumulated in the sample (see SI for more details) as a function of microstructure (orientation and chemistry). In general, these accumulation rates were in line with expectations based upon the spall strength values and the areas under the damage curves presented in Figure 5.5. At lower impact velocities pure Mg displayed the highest damage accumulation rate, while the single crystal [0001] displayed the lowest damage accumulation rate. At higher impact velocities, the two AZ31B rates fell on either side of the pure Mg rate, and the single crystal rates are similar, as expected from examining Figure 6. However, we note two interesting features. First, while the lower velocity AZ31B case seems at first glance to have greater damage than the single crystal cases, the rate of damage accumulation is in fact in line with the $[11\bar{2}0]$ and $[1\bar{1}00]$ orientations. This suggests that, while AZ31 B experiences onset of spall damage very quickly, likely due to a high number of potential nucleation sites, the rate of void growth from that point onward is not notably greater than the $[11\bar{2}0]$ and $[1\bar{1}00]$ orientations. Second, although these damage accumulation rates were fit with linear slopes, it is apparent from Figure 6A that the rate of damage accumulation is not always linear. The [0001], $[11\bar{2}0]$, and pure Mg cases, in particular, are poorly approximated by a single, linear damage

growth rate. There are clear periods of accelerated and reduced growth, suggesting that the rate at which the damage plane grows fluctuates as a function of time and microstructure.

In addition to this examination of damage plane growth rates, the high spatial resolution in this study ($1.6\ \mu\text{m}$) allows the identification and calculation of individual void growth rates from the X-ray images. However, we also note the limitations of this measurement due to void layering in the through thickness direction, uncertainty in void shape in the through thickness direction, and the possibility of voids merging in the through thickness direction before this process can be visually identified in the visible (two-dimensional) plane. Given these limitations, an example of void growth rate calculation is provided in Figure 5.7, where a single void from Figure 5.2 is identified and tracked in each image before it coalesces with neighboring voids (see SI for further details). This results in an estimated void growth rate of roughly $7000\ \mu\text{m}^2/\mu\text{s}$. This void tracking process was repeated for six different voids at different locations across the sample (see SI). The average void growth rate was found to be roughly $13,000\ \mu\text{m}^2/\mu\text{s}$, with a standard deviation of about $5,000\ \mu\text{m}^2/\mu\text{s}$. We note that the growth rates fluctuate, both between voids and (in some cases) across time for each void. This may partially be the result of uncertainties in the measurement, as noted above. However, it may also be due in part to the void growth rate not being constant across the damage plane or throughout time. This is an important observation to make, as many currently used damage models implement a single void growth rate function for all voids across a sample [241, 242, 244]. While these calculations do require assumptions of negligible tilt and void layering, as discussed above, this estimate is the first time such a rate has been experimentally quantified. Using the data extracted from the in-situ images, one could implement either a single averaged void growth rate, or implement a distribution of void growth rates (across space and/or time) extracted from multiple void measurements.

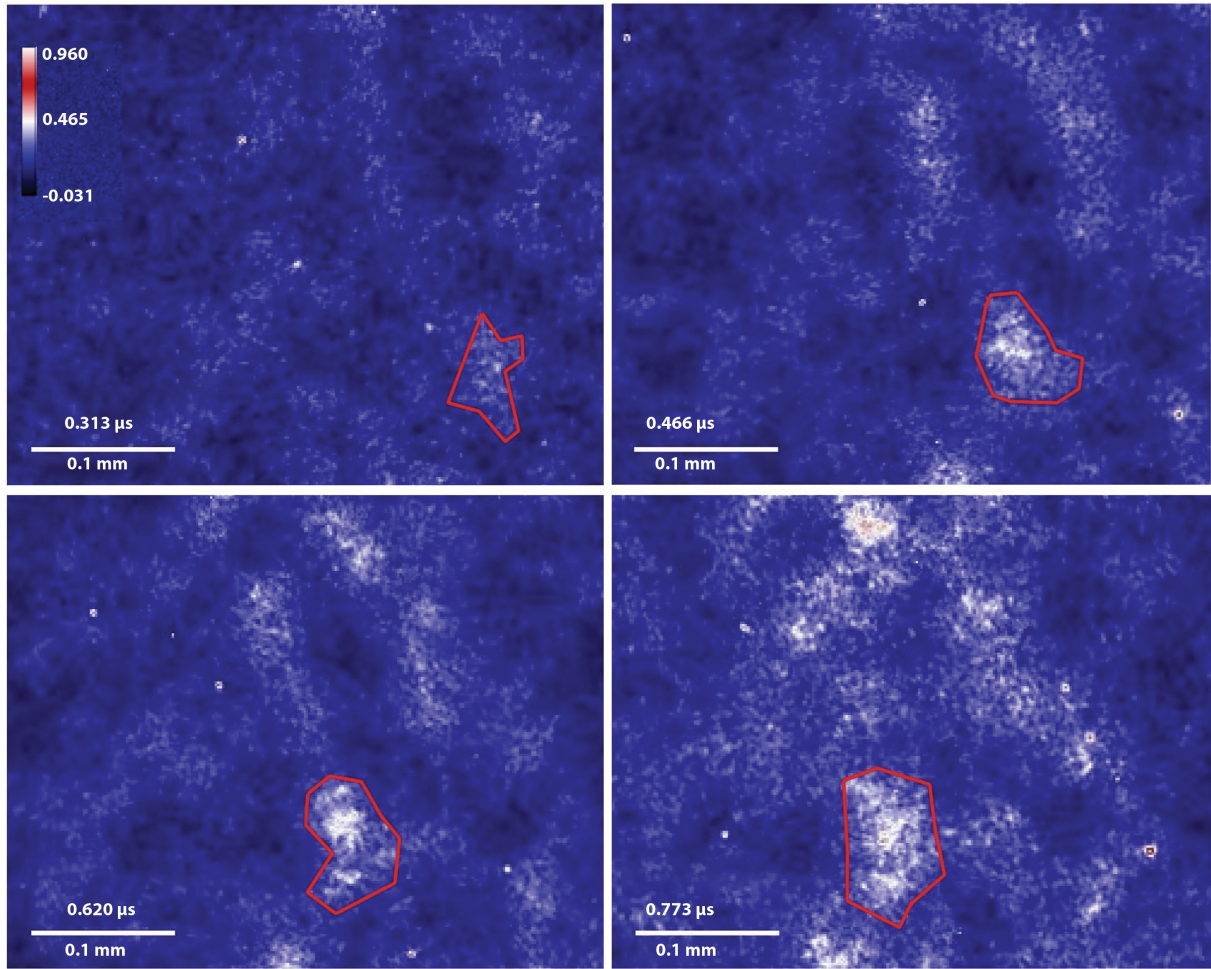


Figure 5.7. A close up view of a void chosen from the polycrystalline Mg sample for tracking. Impact in this sample occurred at $0.4 \text{ mm } \mu\text{s}^{-1}$, with the full sample shown in Figure 5.2 in the main text. The void is tracked over the first four frames, and the area encompassed by the void is outlined in red. We note that the spatial resolution of these images is $1.6 \text{ } \mu\text{m}$. The intensity scale bar is in arbitrary units, consistent with the images shown in Figure 5.2.

5.3 Discussion

In this work, in-situ absorption contrast imaging was used in plate-impact spall experiments to study time-resolved, high-fidelity void and damage evolution in Mg with varying microstructures. These experiments captured the time evolution of void shape and morphology in a spall plane in metals for the first time at such fine spatial resolution. Analysis of the data from these experiments qualitatively and quantitatively showed the following: 1) At low impact speeds, spall strength increased and the total void damage decreased in the order of polycrystalline pure Mg, AZ31B, $[1\bar{1}00]$ and $[11\bar{2}0]$ and $[0001]$ magnesium; 2) Void distribution, shape, and growth direction varied widely from one microstructure to another; 3) Spall strength alone was not an adequate indicator of accumulated voids; and 4) The void damage profile began to shift from Gaussian to bimodal as a function of time in the polycrystalline microstructures.

This data can be used to evaluate and improve the accuracy of current analytical void-based damage models, which generally require the parameterization of several terms associated with specific materials and loading conditions to adequately represent and predict damage. These terms have previously been informed by velocity-time data obtained from the free surface of the material, porosity analysis from recovered samples, or few-frame or low-resolution time-resolved x-ray imaging, which may fail to capture the relevant physics due to not being high-resolution or time-resolved. With the work performed here, it is now possible to refine these models through direct experimental measurement of parameters such as early-stage distribution, growth rates, and shape evolution of both individual voids and accumulated damage. We suggest that the intended use for the technique shown herein should be in conjunction with the previously mentioned traditional techniques, including both pre-experiment and post-mortem characterization (*e.g.* high resolution static x-ray tomography in both cases, and electron microscopy in the latter).

We highlight several unique contributions that this technique can make. Our results make it clear that damage growth is not always linear in nature, meaning that growth rates can fluctuate in a way that requires time-resolved data to capture properly. This is true of

not only growth rates, but also of void distribution, which was shown to shift throughout the process of damage evolution. More traditional techniques, such as post-mortem characterization, do not capture these time-dependent details. Nor do current damage models, which use first order approximations for growth rate and Gaussian approximations for void distribution. While post-mortem characterization has proven useful for estimating void nucleation sites [262–264], we suggest that the time resolved technique shown here can add confidence to these inferences, particularly when paired with damage models. We also suggest there is value in such time resolved measurements, particularly in very high energy and destructive contexts where recovery is not possible. Furthermore, we expect that for materials with more complex microstructures than those examined herein, the nonlinear, time-varying effects we see will worsen, resulting in increased modeling difficulty which could be mitigated with time resolved measurements.

It is similarly important to note that while this data provides information about quantitative evolution of damage in the samples, it does not offer direct insights regarding the exact deformation mechanisms that lead to the varying behaviors. Coupled with improved computational models and current analysis techniques (*e.g.* velocimetry and post-mortem characterization), we suggest that this data will lead to new mechanistic insights to spall failure and void nucleation and growth processes. Additionally, we expect that as the beam energy at synchrotrons is increased, other metals of interest will become accessible for this type of examination.

5.4 Materials and Methods

5.4.1 Materials

Single Crystal Magnesium

Single crystal magnesium samples were obtained from Princeton Scientific, in the form of discs nominally 10 mm diameter by 2 mm thick. Three orientations were chosen, $[0001]$, $[1\bar{1}00]$, and $[11\bar{2}0]$, with these directions aligned with the through-thickness direction of the sample to within one degree. Purity was specified as at least 99.99% for all samples.

Single Crystal Magnesium

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Polycrystal Pure Magnesium and AZ31B

Polycrystalline magnesium and AZ31B samples were machined from plate stock such that the shock direction was along the plate through thickness direction, in an 8 mm diameter by 1.6 mm thick disc format. The pure magnesium plate was hot rolled, and the AZ31B plate was a commercially pure plate in the stress-relieved H24 condition. The SI includes information on the chemistry of each material.

Light optical microscopy (LOM) and electron backscatter diffraction (EBSD) were performed for both the pure Mg and AZ31B materials in order to produce a detailed microstructural analysis. Samples for this analysis were prepared using standard metallographic techniques. They were mechanically ground from 240 to 800 grit, then polished using $0.3\text{ }\mu\text{m}$ colloidal alumina, followed by electro-polishing. This polishing of the EBSD samples was done with a 60% ethanol and 40% phosphoric acid mixture at room temperature, using 3V for approximately 10–15s. Samples were then rinsed with methanol, followed by immersion in a 10% nitric acid and water mixture. Finally, the sample surface was thoroughly cleaned with methanol. The EBSD data was acquired using a Philips XL30 field emission gun (FEG) scanning electron microscope (SEM) and analyzed using software by EDAX.

5.4.2 Plate Impact Experiments

Shock compression experiments were performed on multiple samples at the Dynamic Compression Sector (DCS) at the Advanced Photon Source (Argonne National Laboratory, IL). Further details of the experiments are included in the SI. In brief, a gas-gun was used to launch

a projectile with a flyer-plate into each magnesium sample, driving compression which was then followed by spall fracture. The polycrystalline samples were impacted by a magnesium flyer-plate, half the sample thickness. The single crystal samples were impacted by a 6061 aluminum flyer plate, 1.6 mm thick. Both types of flyer-plate were backed with lexan, to provide support for the flyer-plate during launch while allowing an almost full release. We note that the presence of the polycarbonate backing (see Figure 5.1b) reduces the tension generated in the spall plane, and thus a full release is not achieved. However, experiment parameters were chosen to ensure that spall would still be generated. A PDV probe was placed behind the sample, to measure the rear free-surface velocity. X-ray pulses were passed through the sample (normal to the loading direction) every 153 ns, and captured by a detector bank consisting of a scintillator, intensifier, and multiple cameras. This allowed a total of eight x-rays to be recorded, with a field of view approximately 1.7 mm by 1.7 mm and a spatial resolution of roughly 1.6 μm . The sample was placed in the beam to image the area where spall was expected to occur. For more detail we refer to works that have used a similar experimental setup at this facility [250, 254, 265]. The raw x-ray images were processed in ImageJ and MATLAB. Image correction was first performed, consisting of normalization using accompanying white and darkfield images for each shot, followed by an alignment correction of each camera relative to camera 1 using a reference grid, and finally a straightening correction with respect to the window edge to orient the target relative to the gun barrel, and thus the spall plane is vertical. Each set of images associated with a single experiment therefore has a consistent orientation.

Analysis

Once corrections were applied, analysis to quantify void distribution and porosity as a function of time was performed in MATLAB. Each 1024×1024 pixel image was sliced into a number of vertical ‘bins’. The intensity data was averaged vertically over each bin, resulting in a $1 \times \text{number of bins}$ sized vector representing the averaged intensity values across the horizontal width of the sample. The chosen bin size was varied to examine the effect on the resulting data,

and was found to coarsen the data and remove details as the bin size was increased. However, the overall trends in the data did not change with the bin size. Using this study, a bin size of two pixels was chosen, in order to retain a high level of detail. The averaged intensity curves were plotted together for each experiment (see Figure 5.5). To account for frame-to-frame variations in intensity, the intensity curves were normalized with respect to the flattest (least changing) portion of the curve, outside of the spall damage region where we assume the x-ray path length through the sample was constant - as such this portion undergoes little density variation during the course of the experiment. All times are given with respect to impact, which is defined as time zero.

In the analysis of void distribution via intensity averaging, we assumed a negligible effect on intensity measurements from tilt. The images captured are a two-dimensional representation of a three-dimensional space, and so it might be expected for there to be some contribution from void layering in the through thickness direction on the identifiable edges of the visible voids. We expect that this will introduce some additional uncertainty and fluctuation in rate calculations when tracking individual voids and acknowledge the limitations inherent in the measurements. However, this technique provides the first direct experimental measurement of time-resolved evolution of voids, which can be used to directly estimate parameters such as distribution and growth rate for the first time, despite such through-thickness limitations.

5.5 Supplemental Information

5.5.1 Further Experimental Details

Further information regarding sample composition and impact experiments are included here. Table 5.1 shows a detailed breakdown of the chemistry of the polycrystalline samples, data reused from Ref. [39] with permission of author. Further details of the sample material properties can also be found in Ref. [39]. In Table 5.2 we include a list of the experiments performed, including impact velocity and the timing of the first x-ray relative to sample impact.

Table 5.3 contains detailed information regarding the values used to calculate spall strength in the single crystal experiments. Note that sound speeds were measured using the standard pulse echo method. The PDV setup used a standard homodyne configuration, using a 1550 nm laser and a standoff from the sample of around 3 mm, with a collimating probe sourced from AC photonics (glass, roughly 1.2 mm diameter, with a 0.4 mm spot size). PDV data was reduced using the SIRHEN package, written by Dan Dolan (SNL).

Tilt was taken into consideration by tracking the motion of the rear free surface over the first few frames, which gave no indication of substantial impact from tilt. While no formal tilt diagnostics were performed on this experimental setup, due to limitations in target size and setup at DCS, tilt has previously been measured on a very similar setup through the use of multiple PDV probes and the x-ray diffraction configuration at DCS. This measured tilt was on the order of 1-2 mrad.

5.5.2 Damage Growth Rate

In Figure 5.8 below is shown the calculated rates of damage plane growth, calculated by fitting linear slopes to the curves in Figure 6 in the main text. Table 5.4 lists the slope values.

The spatial resolution in this work ($1.6 \mu\text{m}$) allows the identification and tracking of individual voids, with some caveats and limitations due to uncertainties regarding through-thickness imaging and tilt. MATLAB was used to draw a polygonal region of interest encompassing the area of the tracked void. This same void was then identified in subsequent images, and new regions of interest were drawn, enabling calculation of the growth rate of the area encompassed by the void up until the point when the tracked void coalesces with another void. The area of the single void outlined in Figure 7 in the main text is calculated to estimate a void growth rate of roughly $7000 \mu\text{m}^2/\mu\text{s}$, averaged across the first four frames.

The areas calculated by tracking multiple voids across the sample shown in Figure 2 in the main text are shown in Figure 5.9. We note the shifting slopes, corresponding to shifting void growth rates, both from void to void and across time. The growth rates are found to have a range

of roughly 7,000-19,500 $\mu\text{m}^2/\mu\text{s}$. This corresponds to a average void growth rate, across space and time, of 12,933 $\mu\text{m}^2/\mu\text{s}$, with a standard deviation of 4,968 $\mu\text{m}^2/\mu\text{s}$.

5.5.3 Additional Absorption Contrast Images

Several figures from the main text included images with brightness adjustments in order to more easily identify and compare void morphology. We include here in Figure 5.10 these images without brightness adjustments, displayed with a consistent intensity scale.

Additional sets of images of interest which were not included in the main text are included here as well. In Figure 5.11 and Figure 5.12 we show the images from two experiments of similar microstructure which were repeated under similar impact conditions, highlighting the similarity of the void morphology and the repeatability of our results. Note that further intensity normalization was performed for consistency between experiments for the quantitative analysis shown in Figure 5.13 below, as was the case in the damage integration plots shown in the main text.

5.5.4 Discussion on Uncertainty

There exist several sources of uncertainty and error in these types of experiments which should be mentioned for completeness. Certain natural and unavoidable experimental variations exist, such as sample variability, exact impact velocity, and inherent intensity differences from camera to camera. Every effort was made to account for these variations when possible, including normalization of intensity values before quantitative comparisons, thorough sample characterization, and meticulous documentation. In order to confirm repeatability, two experiments were repeated under similar conditions. The spall strengths calculated from these repeat experiments can be found in Figure 5 in the main text. Although the loss of the imaging from the first $[1\bar{1}00]$ shot (shot 22-2-035) prevented damage comparisons in that case, the processed and normalized damage comparison from the repeated experiment in shots 22-2-039 and 22-2-041 are included in Figure 5.13 below. Despite the unavoidable, natural fluctuations from one experiment to

another, we find good agreement in repeat experiments.

In addition to experimental uncertainty, we explore our analytical treatment to ensure that our averaging techniques are not introducing any fundamental alterations of the data. As described in the Methods section in the main text, images were averaged vertically across the width of the image in order to produce the intensity and damage area plots in the main text. Differing bin sizes were explored for this analysis, and it was found that increasing bin size smoothed the data and resulted in a loss of detail. A low bin size of two pixels was therefore chosen to retain a high level of detail and avoid altering the data.

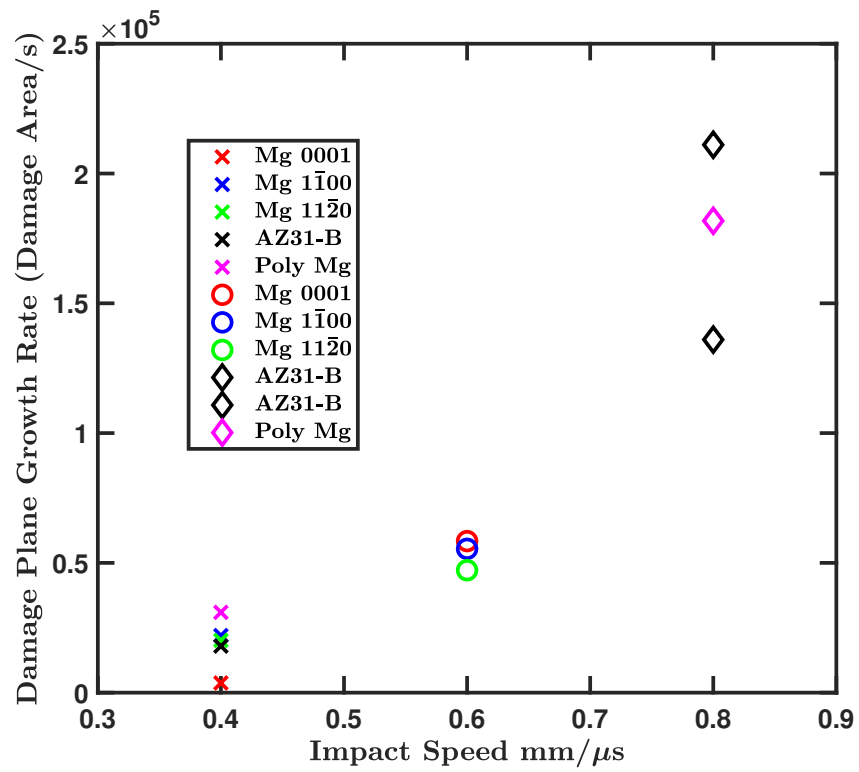


Figure 5.8. Damage plane growth rate as a function of microstructure and impact speed, calculated by fitting a linear slope to the integrated intensity over time plots shown in Figure 6 in the main text.

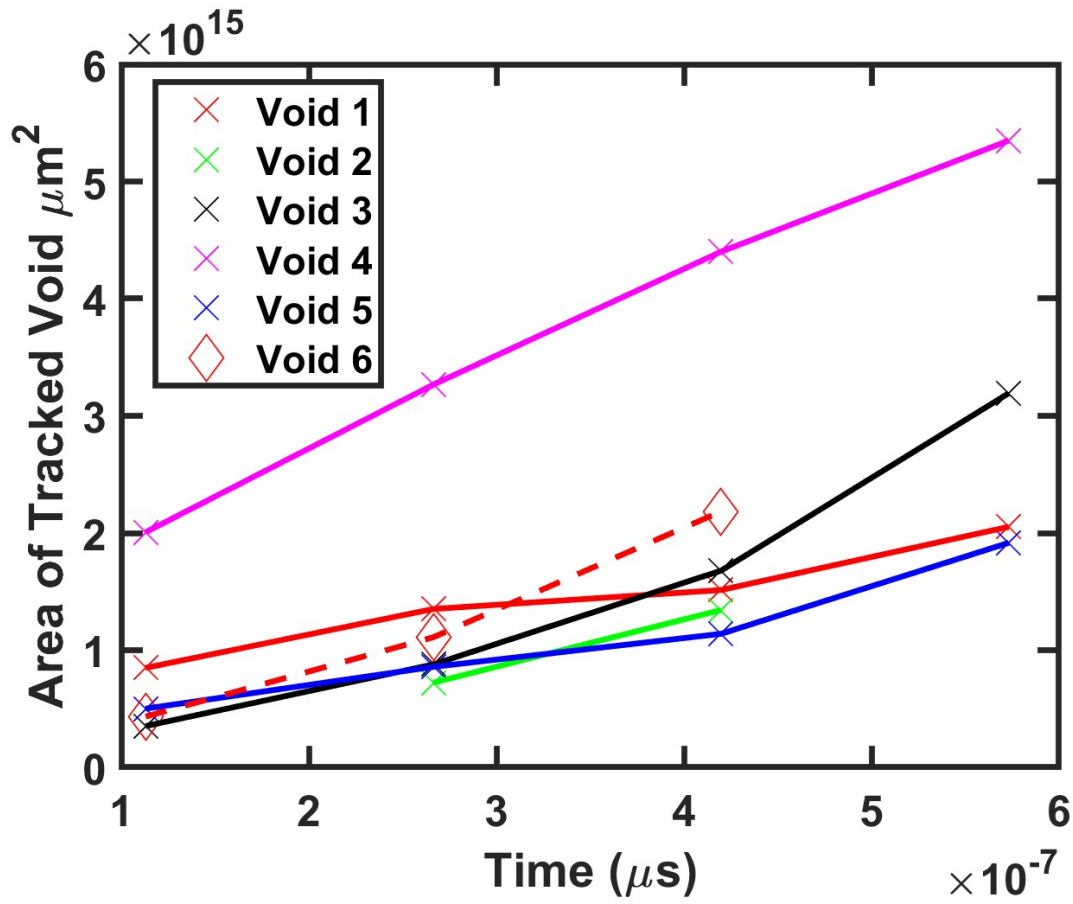


Figure 5.9. Tracked void areas as a function of time, the result of the analysis technique performed in Figure 5.7 in the main text, repeated for multiple different voids across the sample shown in Figure 5.2 in the main text. The growth rates (averaged across time), respectively, are found to be 7,028, 10,864, 16,589, 19,519, 8,264, and 15,331 $\mu\text{m}^2/\mu\text{s}$.

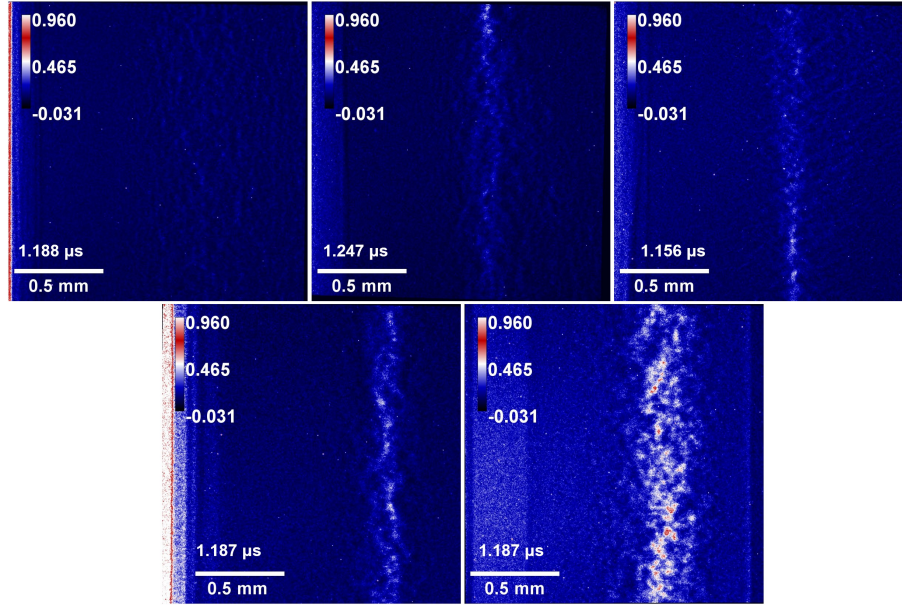


Figure 5.10. A comparison of x-ray images from different samples at similar times, in which no brightness adjustment has been performed, in which all images are displayed with the same intensity scale. A) single crystal $[0001]$, B) single crystal $[11\bar{2}0]$, C) single crystal $[1\bar{1}00]$, D) AZ31-B and E) pure magnesium. Impact speed for all samples shown was $0.4 \text{ mm } \mu\text{s}^{-1}$.

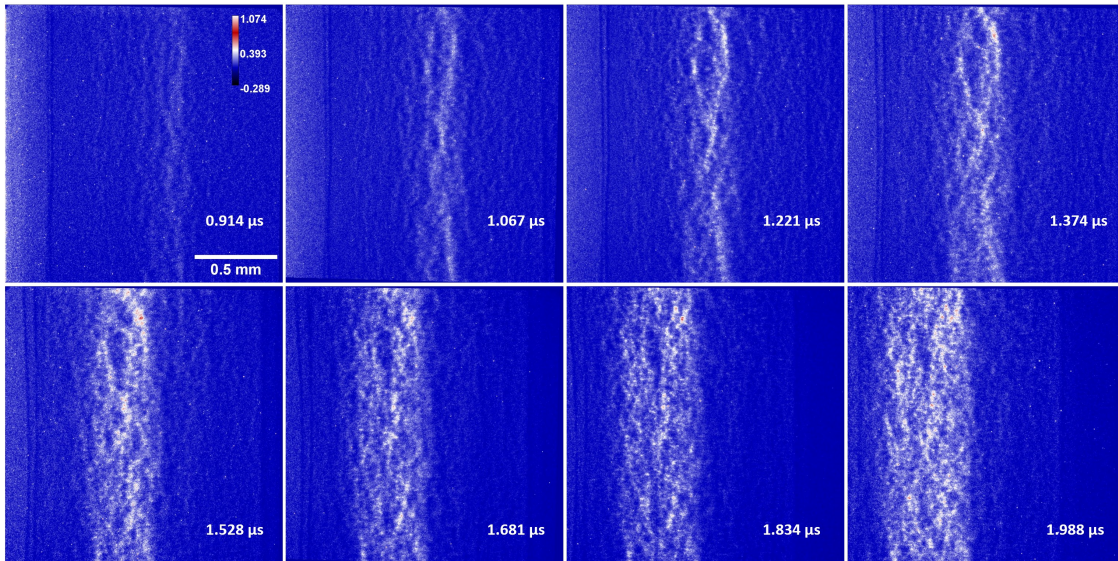


Figure 5.11. A comparison of x-ray images from a single crystal $[11\bar{2}0]$ oriented sample impacted at $0.6 \text{ mm } \mu\text{s}^{-1}$. Corresponds with shot 22-2-039, the red damage curve in Figure 5.13

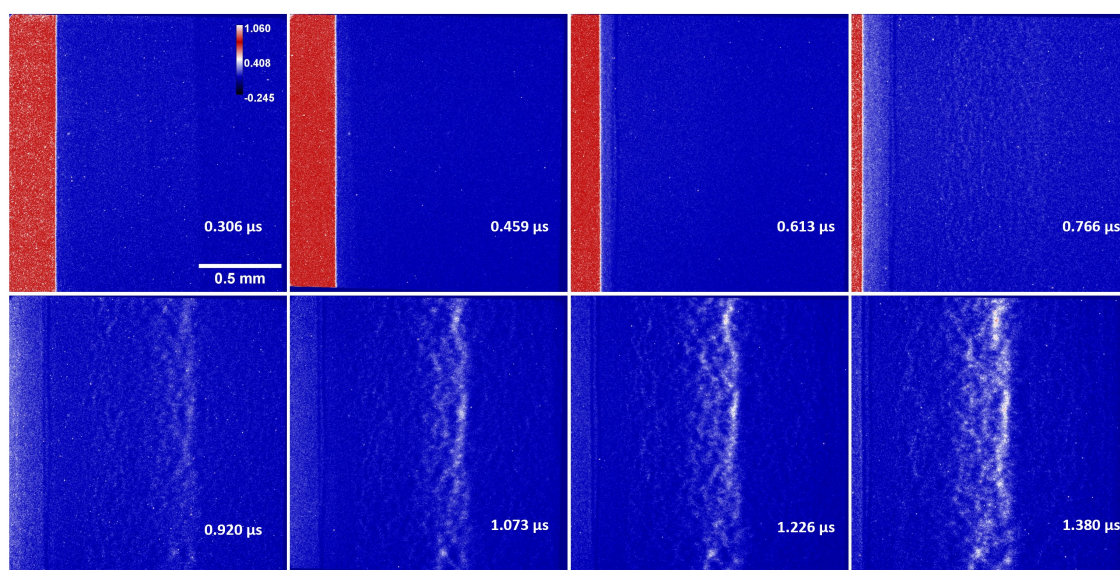


Figure 5.12. A comparison of x-ray images from a single crystal $[11\bar{2}0]$ oriented sample impacted at $0.6 \text{ mm } \mu\text{s}^{-1}$. Corresponds with shot 22-2-041, the blue damage curve in Figure 5.13

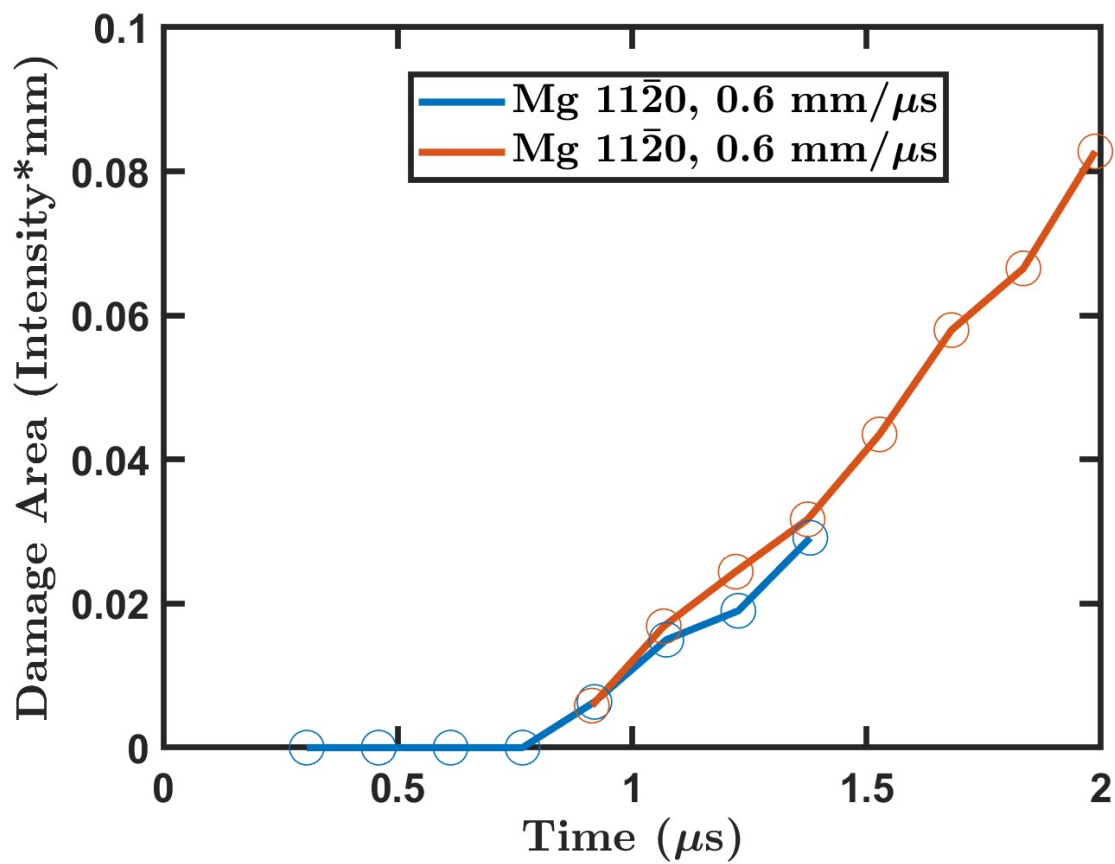


Figure 5.13. A damage comparison between experiments run under similar condition, on a single crystal sample of $[1\ 1\ \bar{2}0]$ orientation, impacted at $0.6\ \text{mm}\ \mu\text{s}^{-1}$.

Table 5.1. Chemistry of the polycrystalline magnesium samples used in this study.

Sample	Al	Ca	Mn	Zr	Zn	Sn	Si	Pb	Cu	Fe
Pure Mg (wt%)	0.0033	0.0016	0.0090	0.0038	0.0350	0.0049	0.0046	0.0085	-	-
AZ31B (wt%)	3.02	-	0.3	-	1.01	0.007	-	-	0.003	0.003

Table 5.2. Summary of the plate-impact experiments.

Experiment	Sample	Impact Velocity ($\text{mm}\mu\text{s}^{-1}$)	Time of First X-ray Relative to Impact (μs)
21-2-017	AZ31B	0.8	0.463
21-2-018	Polycrystalline	0.4	0.113
21-2-019	AZ31B	0.4	0.113
21-2-026	Polycrystalline	0.8	0.462
21-2-027	AZ31B	0.8	0.462
22-2-033	[0001]	0.4	0.881
22-2-034	[0001]	0.6	0.793
22-2-036	[1 $\bar{1}$ 00]	0.6	0.376
22-2-037	[1 $\bar{1}$ 00]	0.4	0.696
22-2-038	[11 $\bar{2}$ 0]	0.4	0.480
22-2-039	[11 $\bar{2}$ 0]	0.6	0.914
22-2-041	[11 $\bar{2}$ 0]	0.6	0.306

Table 5.3. Spall strength relevant parameters single crystal experiments.

Experiment	Sample	Impact Velocity ($\text{mm}/\mu\text{s}$)	δu_{fs} ($\text{mm}/\mu\text{s}$)	C_B ($\text{mm}/\mu\text{s}$)	C_L ($\text{mm}/\mu\text{s}$)	Spall Strength (GPa)
22-2-033	[0001]	0.4	0.307	5.301	6.395	1.41
22-2-034	[0001]	0.6	0.306	5.301	6.395	1.41
22-2-036	[1 $\bar{1}$ 00]	0.6	0.275	3.653	5.169	0.87
22-2-035	[1 $\bar{1}$ 00]	0.4	0.27	3.653	5.169	0.86
22-2-037	[1 $\bar{1}$ 00]	0.4	0.252	3.653	5.169	0.80
22-2-038	[11 $\bar{2}$ 0]	0.4	0.238	4.775	6.108	0.99
22-2-039	[11 $\bar{2}$ 0]	0.6	0.244	4.775	6.108	1.01
22-2-041	[11 $\bar{2}$ 0]	0.6	0.254	4.775	6.108	1.05

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Table 5.4. Damage plane growth rates, extracted from Figure 6 in the main text with a linear slope fit.

Microstructure	Impact Velocity (mm μs^{-1})	Damage Plane Growth Rate (Damage Area/s)
[0001]	0.4	3,741.75
[0001]	0.6	58,390.08
[1100]	0.4	22,003.63
[1100]	0.6	55,418.64
[1120]	0.4	17,933.91
[1120]	0.6	47,169.84
AZ31B	0.4	17,933.91
AZ31B	0.8	211,067.41 and 136,004.11
Polycrystalline	0.4	30,948.34
Polycrystalline	0.8	181,776.81

Nicholas Boechler, and Saryu Fensin. In situ measurement of damage evolution in shocked magnesium as a function of microstructure. Sci. Adv.9,eadi2606(2023).DOI:10.1126/sciadv.adi2606. The dissertation author was the primary author of this paper. Authors: Brianna MacNider, David Jones, Jesse Callanan, Matt Beason, George T. Gray III, Dana M. Dattelbaum, Nicholas Boechler, Saryu Fensin.

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Chapter 6

Conclusions and Future Work

While fully realizable high strain rate metamaterials remain a complex and difficult problem with further challenges to conquer, in this work we have taken steps toward this goal and made significant progress in furthering the tools required to get there. We have demonstrated a comprehensive, multi-level, 1D inverse design methodology for targeted nonlinearities which incorporates low strain rate dynamics. Through this, we enable inverse design for nonlinear, spatially varying wave effects, tackling one important challenge on the path toward high strain rate metamaterials. We furthermore explored the extension to intermediate strain rates in architected materials, providing insight into critical differences between strain rate regimes that must be better understood to incorporate the required physics into inverse design problems. Finally, we have investigated failure mechanisms at high strain rates with an in-situ examination of spall void growth, enabling better characterization and modeling of such processes. The insights provided through the intermediate and high strain rate experimental work will be key in extending modeling and inverse design efforts into these regimes.

The work herein has provided a critical step toward future work to further extend capabilities. Below we outline a non-comprehensive list of a few promising areas for future investigation.

- The extension from 1D to 2D in both topology optimization and DEM implementation, incorporating the effect of coupled shear.

- The inclusion in topology optimization of viscoelasticity and/or targeted damping behavior.
- The inclusion in both topology optimization and DEM of effects often seen at high strain rates and deformations, such as plasticity.
- An investigation of the validity of representing high strain rate shocks in a spring-mass DEM model.

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