ARCHITECTED MATERIALS: SYNTHESIS, CHARACTERIZATION, MODELING, AND OPTIMAL DESIGN

This Focus Issue of the Journal of Materials Research contains articles that were accepted in response to an invitation for manuscripts.

Introduction

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I. INTRODUCTION

Architected materials are multiphase and/or cellular materials in which the topological distribution of the phases is carefully controlled and optimized for specific functions or properties. Nearly two decades of research has resulted in the identification of a number of topologically simple, easy to fabricate, well-established structures (including honeycombs and truss lattices), which have been optimized for specific stiffness and strength, impact and blast protection, sound absorption, wave dispersion, active cooling, and combinations thereof.

Over the past few years, dramatic advances in processing techniques, including polymer-based templating [e.g., stereolithography, photopolymer waveguide prototyping, and two-photon polymerization (2PP)] and direct single- or multimaterial formation (e.g., direct laser sintering, deformed metal lattices, 3D weaving, and knitting), have enabled fabrication of new architected materials with complex geometry and remarkably precise control over the geometric arrangement of solid phases and voids from the nanometer to the centimeter scale.

The ordered topologically complex nature of these materials and the degree of precision with which their features can now be defined suggest the development of new multiphysics and multiscale modeling tools that can enable optimal designs. The result is efficient multiscale cellular materials with unprecedented ranges of density, stiffness, strength, energy absorption, permeability, chemical reactivity, wave/matter interaction, and other multifunctional properties, which promise dramatic advances across important technology areas such as lightweight structures, functional coatings, bioscaffolds, catalyst supports, photonic/phononic systems, and other applications.

Some of the most exciting recent developments in this field are the exploration of size effects in the development of nano-architected materials with superior combinations of properties, the investigation of geometrically complex unit cell architectures that enable nonlinear effective mechanical response from linear–elastic materials, novel manufacturing approaches with increased resolution and scalability, and improved design optimization tools. Here, we briefly review some recent progress in these areas and conclude with some thoughts about opportunities for future development. The collection of articles in this focus issue is a wonderful exposure to some of the latest original studies in this field.

II. RECENT PROGRESS IN THE FIELD

A. Size effects in nano-architected materials

Accurate control of chemistry and microstructure has been the established route for materials development for centuries. The design of architected materials, whereby the geometrical arrangement of matter is optimized for specific combinations of properties, provides an alternative approach. This approach has been exploited—primarily for mechanical properties—for the past two decades and has resulted in significant colonization of white space in material property maps (Ashby charts). For example, following principles of civil engineering, matter can be efficiently arranged along load paths in structural architected materials, thus resulting in excellent specific strength and stiffness.

In a periodic architected material, the unit cell size is much smaller than the scale at which loads (mechanical, thermal, etc.) are applied, so that the material can be

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looked at as a homogeneous effective medium. Under these conditions, the effective properties of the architected materials are a function of topology (the way in which the matter is arranged in the unit cell) and constituent(s) material properties (the properties of the solid material(s) of which the architected material is made). Often (but not always), these contributions are multiplicative, i.e., $p_{\mathrm{eff}} = f(p_{0i})\cdot g(\mathrm{topology})$, with $f(p_{0i})$, a function only of the constituent material(s) properties, and g(topology), a purely geometric function. For more details, please refer to Refs. 1–3 and references within.

In much of the published work on architected materials, the smallest geometrical scale (e.g., the truss diameter in a lattice material) is still much larger than the microstructural scale (e.g., the grain size in a metallic lattice); as a result, $f(p_{0i})$ is independent on scale, and two geometrically self-similar architected materials with different scales will have the same effective properties.

This scale independence breaks down when the smallest geometrical scale approaches the microstructural scale. Under these conditions, beneficial size effects can be exploited to increase $f(p_{0i})$ and hence develop architected materials with effective properties that are superior to those attainable with size-independent materials. See Ref. 4 and references within for a recent overview of work in this area. This approach has been demonstrated successfully for high specific strength in a number of studies. Consider a lattice material (e.g., an octet lattice). When subjected to macroscopic mechanical loads, the lattice may fail by three mechanisms: plastic flow at the strut level, fracture of the struts, or elastic buckling (whether at the strut level or at longer wave length). All three mechanisms can be controlled by size: (i) The yield strength at the strut level can be increased by reducing the grain size (Hall–Petch effect) and nanoscale grain size is easier to process on micron-scale objects than in bulk solids; as the strut size approaches the nanoscale, dislocation starvation-based size effect kick in and strength can be further increased. (ii) Fracture is controlled by the presence of flaws in the strut; as the strut diameter is reduced, so is the largest flaw size, down to a point where the strain energy release rate upon loading is insufficient to drive a crack and the theoretical strength is attained. (iii) Finally, buckling can be delayed by hierarchical designs, which require several length scales (and hence the smaller the strut diameter, the more hierarchy we can obtain for a given macroscopic lattice size).

Notice that in the absence of beneficial size effects, reducing the unit cell size of a cellular material (including lattices) results in a decrease in fracture toughness proportional to the square root of the unit cell size.[1] In principle, this phenomenon can be compensated by exploiting strut-level strengthening at the nanoscale, allowing nanoscale lattices to retain appreciable strength[5]; experimental verification of this concept is still lacking. Ultimately, to increase fracture toughness, mechanisms for energy absorption and/or crack deflection must be introduced. Complex unit cell architectures with hierarchy and/or shell-based (as opposed to truss-based) designs can help in this regard, although this is still a current area of research.

While most of the research efforts to date have focused on exploring size effects in strength, there are other mechanical properties that can benefit from scale reduction: for example, there are early indications that energy absorption in nano-architected composites can improve when the unit cell is shrunk to the nanoscale.[6] Thermal properties can also be improved: for example, the effective thermal conductivity of a lattice is proportional to the thermal conductivity of the strut material, which can be reduced as the diameter of the strut approaches the nanoscale, thus increasing phonon scattering at the strut surface. This is also a current area of research.

Finally, reducing the unit cell size of an architected material to the micro- and nanoscale allows interaction with wave phenomena with wave length comparable (or larger) than the unit cell size; this is the main principle behind electronic and optical metamaterials (for EM waves) or acoustic metamaterials (for acoustic/elastic waves), including phononic crystals. Several phenomena in wave-based metamaterials have been heavily investigated over the past two decades.[7–11] Nonetheless, many exciting frontiers still exist, with optical cloaking being probably the most notable example.

B. Nonlinear architected materials

Since the properties of architected materials are governed primarily by their geometry, materials with tunable functionality can be created by incorporating internal mechanisms capable of altering their spatial architecture in situ. In particular, one recent finding is that the dramatic changes in structural geometry induced by large deformations and mechanical instabilities may lead to strongly nonlinear relations between macroscopic stresses and strains, even if the material remains in the near-linear regime. Symmetric slender elements can undergo buckling instabilities that result in strong but reversible geometric nonlinearities under precisely designable loading conditions. Moreover, many slender elements feature two stable states connected by a rapid and irreversible ‘snap-through’ instability. For elastic materials, the geometric reorganization triggered by these phenomena is both reversible and repeatable and occurs over a narrow range of applied load. Therefore, architected materials created by assembling these nonlinear building blocks incorporate a range of completely new functionalities.

Architected materials often consist of periodic networks of beams, which are known to buckle under axial compression. When deforming such structures in the elastic regime, buckling may trigger dramatic homogeneous and reversible pattern transformations.[12,13] Recently, such instabilities have been exploited to design architected materials with tunable negative Poisson's ratio and effective negative swelling ratio[14] structures capable of switching between achiral and chiral configurations,[14] soft actuators[15] and robots,[16] materials with tunable optical properties,[17,18] and dynamic response.[19–22]

Elastic beams not only buckle but may also snap between two different stable configurations, retaining their deformed shape after unloading. As bistable elastic beams can lock in most of the energy provided to the system during loading, they have been recently used to create fully elastic and reusable energy-trapping architected materials.[23–25] Moreover, the ability of bistable beams to release stored elastic energy has been exploited to overcome both dissipative and dispersive effects to allow the propagation of mechanical signals with a large amplitude in soft systems made of dissipative materials.[26]

Exploiting instability in solids and structures has offered new opportunities for the design of architected materials with enhanced functionalities. In the future, some of the exciting directions include coupling the mechanics of architected materials with other phenomena, such as adhesion, friction, and flow; incorporating sensing and control functionalities into architected systems to design materials capable of autonomously responding to changes in the surrounding environment; and developing architected materials for which topological properties bring new phenomena.

C. Novel fabrication methods

Architected materials are typically geometrically complex three-dimensional structures which have critical features ranging over orders of magnitude in size-scale, potentially from the nanoscale to the macroscale. To further compound the complexity, in many cases, they are also comprised of multiple material constituents. As a result, fabrication of these unique metamaterials at scale is extremely challenging and historically, this has been a reason for their limited adoption. Prior to the fabrication advancements of the last decade, architected materials were relegated to simple designs or theoretical studies only.

Advanced manufacturing and fabrication methods have developed rapidly in the last decade with many commercially available tools as well as more sophisticated custom capabilities in academic and research institutes. Core to these fabrication methods is the concept of adding material in bottom-up fashion as opposed to material removal. This allows for a radically improved ability to generate complex structures with internal features at multiple size-scales.

There are many methods for adding material to build up a complex structure. Among the most flexible are light-based processes such as stereolithography, projection microstereolithography (PμSL),[27] continuous liquid interface printing,[28] self-propagating polymer waveguides,[29] and 2PP.[30] While some of these are available commercially, many are customized systems specifically tuned for architected materials. Additionally, these light-based methods all utilized photopolymers as their fundamental feedstock material, but researchers throughout the world have also made advances in novel feedstocks such as preceramic polymers[31] and nanoparticle-loaded resins.[32] Combined with advanced post-processing technologies, this has led to the ability to convert the initial polymer structures to alternate materials such as ceramics and metals. The critical small-scale feature sizes required for much of the enhanced performance of architected materials can be achieved with 2PP (nanoscale), PμSL (micro- to macroscale), and self-propagating wave guides (micro-to macroscale). Finally, more recently, some of these methods have been able to generate multimaterial structures with mixtures of metals, ceramics, and polymers in a single structure.[33]

In addition to light-based photocuring methods, there are extrusion-based fabrication processes which are also well suited to architected materials. The most common method is fused deposition modeling which is widely available commercially. This technique works by extruding a thermoplastic filament through a heated nozzle thereby softening and reforming material. More flexible are custom direct write extrusion methods which rely on the design of a material's rheology, so that it will flow through a nozzle and gel, holding its shape upon exit of the nozzle. Paramount to this approach is the synthesis of a viscoelastic ink with these shear thinning properties.[34] Through this more flexible process, a wide range of materials can be accessed including thermoset polymers, nanoparticle-loaded inks, sol–gels, and aerogels. Additionally, fine feature sizes have been demonstrated including filaments with diameters in the submicron range[35] while full-scale components approaching meters have also been fabricated.[36] Finally, with multiple nozzles, or printheads, multimaterial capability can be achieved.

There are a wide variety of other methods which hold promise for architected material fabrication including commercially available polyjet systems, other custom droplet generation techniques, laser powder-bed fusion, and electron beam powder-bed fusion, to name a few. While polyjet and droplet generators in general can create moderately small feature sizes and use multiple polymers, laser and ebeam powder-bed fusion are ideal for larger-scale metallic structures.

The past decade has seen significant advancements in highly three-dimensional fabrication methods which have helped to accelerate the research and adoption of architected materials, as you will see in this focus issue. While this has greatly benefited the community, there are still barriers and challenges associated with scale-up of small feature sizes into large structures, mixtures of materials and broadening of material sets in general, and fabrication reliability, tolerances, and qualification.

D. Novel design optimization tools

The increased freedom that these novel fabrication processes provide has created exciting opportunities in design and highlighted the need for efficient and effective design tools for architected materials. This includes not only base material(s) selection (constituent material properties) but also optimizing the geometric properties of the unit cell design.

When the unit cell topology is prescribed, the resulting geometry design problem is a sizing and/or shape optimization problem. This has been widely explored in the design of truss lattices, where optimizing the diameters and angles of truss struts would constitute sizing optimization and shape optimization, respectively. When the considered architected material is relatively simple (topologically speaking), elegant analytical expressions for linear mechanical properties enable rapid optimization and design of truss parameters.[1] In cases where analytical expressions are not available, such as for nonlinear properties, the relatively small number of design variables (strut diameters and/or angles) allows for parameter sweeps to create design tables and property plots, providing ready access to geometry–property relations for the considered topology.[37]

With new fabrication capabilities comes a significantly enlarged design space, and newly desired performance metrics, including those governed by nonlinear mechanics and multiple physics, amplify the need to fully explore this space in search of novel architectures. For complex design problems, it becomes quite challenging to identify the optimal truss lattice architecture a priori, and it is quite possible that the optimal architecture of the material may not even resemble a lattice. For these reasons, topology optimization is gaining significant traction as a systematic design tool for architected materials. Topology optimization seeks to identify the optimal distribution of material(s) across a design domain, which for architected materials design is the unit cell. Its unique ability to add or remove material(s) throughout the design domain means the connectivity of material is continuously evolving throughout the design process. An arbitrary initial design thus has the ability to transform into any number of architectures, such as lattices, minimal surfaces, organic shapes, or any combination thereof. Key to the effectiveness of topology optimization is that the governing mechanics models are embedded within the optimization formulation, and design decisions are driven by formal mathematical programming (see Ref. 38 for a basic review of this process for architected materials).

Although the first studies in topology optimization of architected materials (termed "material structures" at the time) considered truss representations and optimized for elastic properties, including designing negative Poisson's ratio materials,[39] the approach has been extended to continuum representations for a wide range of physics. This has included optimizing/tailoring properties related to coefficient of thermal expansion,[40] thermal conductivity,[41] fluid permeability,[42,43] phononic crystals,[44,45] viscoelastic damping,[46–48] magnetic metamaterials,[49,50] and nonlinear mechanical properties including energy absorption[38,51] and Poisson's ratio under large deformation.[52] See Ref. 53 for a more thorough survey of topology optimization applied to architected materials design.

Equally important to the optimization of physics-based properties is the incorporation of manufacturing constraints and properties within the topology optimization formulation. It is quite clear that the optimal design of a material architecture is dependent on the manufacturing process: a lattice manufactured by 3D weaving will look dramatically different than one fabricated by powder-bed fusion, even when optimized for the same performance property.

Further, even as fabrication processes advance and continue to provide additional capabilities, manufacturing variabilities (flaws) are inevitable and constraints of some form, such as minimum achievable length scales and radius of curvatures, will remain. Significant progress has been made in integrating manufacturing constraints and variabilities in the topology optimization process for the design of robust components, and this work is slowly making its down to the material architecture scale.

The field of topology optimization is undergoing rapid growth, especially due to its natural synergy with additive manufacturing. Significant challenges, however, remain. Among these are the rigorous and computationally efficient integration of nonlinear mechanics, multiple physics, uncertainty, and complex manufacturing constraints within the topology optimization framework at the scales of architected materials and macroscale components, as well as the connection across these scales (ideally with consideration of material microstructure) to realize true multiscale design optimization.

III. CONCLUSIONS AND OUTLOOK

The field of architected materials has seen enormous interest from the academic community over the past two decades. A plethora of articles have been published, primarily on the topics of EM/optical metamaterials and mechanical metamaterials with exceptional specific strength. Novel modeling and optimization tools and fabrication techniques have been recently proposed, significantly opening the complexity of designs that can be realized. Yet, several concepts are still in their infancy.

In particular, over the next two decades, we expect enormous progress in the following areas: (i) Development of architected materials optimized for nonmechanical and/or multifunctional properties, including thermal, electrical, and transport properties. This might have significant applications in scaffolds for biological cell growth and complex material systems for energy production and storage. (ii) Fast and efficient, rigorous topology optimization tools for nonlinear objectives and constraints, and multiphase, multiscale architected materials. (iii) Scalable fabrication techniques that enable fast production of large-scale multiphase architected materials with controlled micro- and nanoscale features. Ultimately, though, for architected materials to find widespread application in the market, it is essential to bridge the gap between fundamental academic research and industrial development. *Manufacturing Foresight*, a NSF and NIST-funded manufacturing think-tank, recently produced a report on Metamaterials Manufacturing with a number of suggestions on this topic (see “A call to action: Manufacturing Architected Materials” in this issue).

ON THE COVER:

Rendering of a look through a lattice of octet trusses. Image courtesy of LLNL.

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