NUMERICAL METHODS IN ENGINEERING SERIES

Topology Optimization Design of Heterogeneous Materials and Structures

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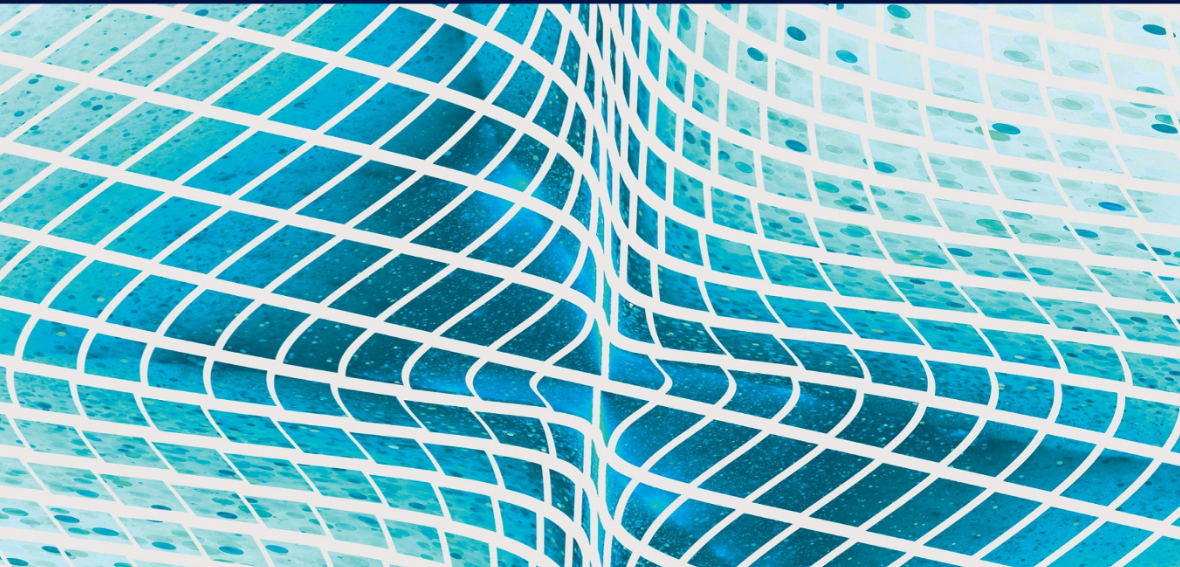

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Contents

Introduction

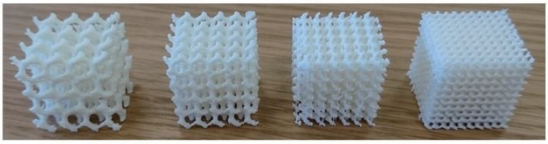
In this Introduction, the background and motivations of the book are presented in section I.1. A literature review on related subjects, including topology optimization methods, material design and multiscale optimization, and fracture resistance design, is presented in section I.2. The outline of the book is presented in section I.3.

I.1. Background and motivations

Topology optimization has been an active research topic in the last decades and has become a subject of major importance with the growing development of additive manufacturing processes, which allow the fabrication of workpieces such as lattice structures with arbitrary geometrical details. In this context, topology optimization (Bendsøe and Kikuchi 1988, Allaire 2012) aims to define the optimal structural or material geometry with regard to specific objectives (e.g. maximal stiffness, minimal mass or maximizing other physical/mechanical properties) under mechanical constraints such as equilibrium and boundary conditions. The key merit of topology optimization over conventional size and shape optimization is that the former can provide more design freedom, consequently leading to the creation of novel and highly efficient designs. With the topology optimization technique, designers can make the best use of limited materials and guide the concept design of various practical structures, especially in automotive and aerospace engineering.

In recent years, there has been an increase in the use of high-performance heterogeneous materials such as fibrous composite, concrete materials and 3D printed materials. Mechanical and physical properties of complex heterogeneous materials are determined, on the one hand, by the composition of their constituents but can, on the other hand, be drastically modified at a constant volume fraction of heterogeneities, by their geometrical shape and by the presence of interfaces. Topology optimization of microstructures can help design materials with higher effective properties while maintaining the volume fraction of constituents or obtaining new properties which are not naturally available (metamaterials). Recently, the development of 3D printing techniques and additive manufacturing processes has made it possible to directly manufacture designed materials from a numerical file, opening routes for new designs, as shown in Figure I.1. It is no exaggeration to say that "additive manufacturing" and "topology optimization" are the best couple made for each other. To this end, systematic and comprehensive research on the topological design of complex heterogeneous materials is of great significance for academic research and engineering applications.

(a)



(b)

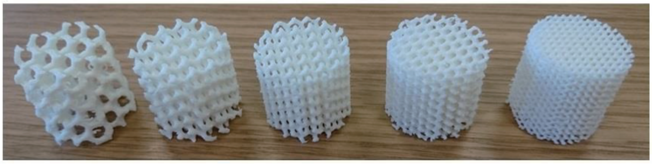
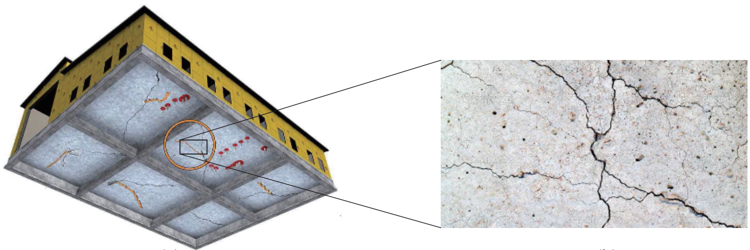


Figure I.1. *3D printed lattice materials: (a) cubic and (b) cylindrical configurations (Mohammed* et al. *2017)*

However, in topology optimization of material modeling, the scale separation is often assumed. This assumption states that the characteristic length of microstructural details is much smaller than the dimensions of the structure, or that the characteristic wavelength of the applied load is much larger than that of the local fluctuation of mechanical fields (Geers *et al.* 2010). In additive manufacturing of architectured materials such as lattice structures, the manufacturing process may induce limitations on the size of local details, which can lead to a violation of scale separation when the characteristic size of the periodic unit cell within the lattice is not much smaller than that of the structure. In such a case, classical homogenization methods may lead to inaccurate description of the effective behavior as non-local effects, or strain-gradient effects may occur within the structure. On the other hand, using a fully detailed description of the lattice structure in an optimization framework could be computationally expensive. One objective of this book is to develop multiscale topology optimization procedures not only for heterogeneous materials but also for mesoscopic structures in the context of non-separated scales.



(a) (b)

Figure I.2. *Damage phenomena in engineering: (a) macroscopic structure; (b) cracks (Nguyen 2015)*

On the other hand, fatigue or failure characteristics of engineering structures are another subject of great concern, as shown in Figure I.2. Microcracking is known to be a significant factor affecting the mechanical properties and the long-term behavior of engineering facilities. The accurate modeling of these phenomena, as well as their coupled effects have received special attention. In addition, topology optimization design of composite materials accounting for fracture resistance is a rather challenging task. It is necessary to improve the fracture resistance of heterogeneous materials in terms of the required mechanical work, through an optimal placement of the inclusion phase, taking into account the crack nucleation, propagation and interaction. However, this research remains relatively unexplored so far due to the following reasons. First, there has been a lack of robust numerical methods for fracture propagation in the presence of complex heterogeneous media until recently, especially when interface effects are presented. Second, these numerical simulation models should be formulated in a context compatible with the topology optimization scheme. For these reasons, there has been very limited research in the literature on topology optimization for maximizing the fracture resistance of heterogeneous materials before the recent works from the author and his coworkers (Xia *et al*. 2018a, Da *et al*. 2018a).

I.2. Literature review

In the following, section I.2.1 provides a brief literature review on the development of topology optimization methods. Section I.2.2 reviews material microstructure design and extension to multiscale topology optimization with or without scale separation. Section I.2.3 presents the newly proposed fracture resistance design framework, by combining the phase field method to take into account the heterogeneities and their interfaces in the material.

I.2.1. *Topology optimization methods*

Over the past decades, topology optimization has undergone a tremendous development since the seminal paper by Bendsøe and Kikuchi (1988). The key merit of topology optimization over conventional size and shape optimization is that the former can provide more design freedom, consequently leading to the creation of novel and highly efficient designs. Various topology optimization methods have been proposed so far, for example density-based methods (Bendsøe 1989, Zhou and Rozvany 1991, Bendsøe and Sigmund 2004), evolutionary procedures (Xie and Steven 1993, 1997), level-set method (LSM) (Sethian and Wiegmann 2000, Wang *et al*. 2003, Allaire *et al*. 2004), hybrid cellular automaton (Tovar *et al*. 2004) and phase field method (Bourdin and Chambolle 2003). All of these methods are based on finite element analysis (FEA) where the design domain is discretized into a number of finite elements. With such a setting, the optimization procedure is then to determine which points of the design domain should be full of material (solid elements) and which void (soft elements), as shown in Figure I.3. According to the update algorithm, these methods can be generally categorized into two groups: density variation and shape/boundary variation. The topology optimization technique has already become an effective tool for both academic research and engineering applications. A general review of various methods and their applications was presented by Deaton and Grandhi (2014). Regarding their strengths, weaknesses, similarities and dissimilarities, a critical review and comparison on different approaches was also given by Sigmund and Maute (2013).

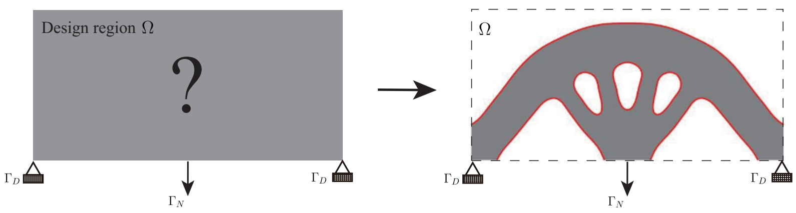


Figure I.3. *Illustration for structure topology optimization*

Level-set method (LSM) is a typical shape/boundary variation approach that maintains the capability of topological change. It describes the structural topology implicitly by the iso-contours of a level-set function. Using the LSM, a fixed rectilinear spatial grid and a finite element mesh of a given design domain can be constructed separately, which allows the separation of the topological description from the physical model. With the merits of the flexibility in handling complex topological changes and the smoothness of boundary representation, the LSM has been successfully applied to an increasing variety of design problems, involving, for example, multi-phase materials (Wang and Wang 2004), shell structures (Park and Youn 2008), geometric nonlinearities (Luo and Tong 2008), stress minimization (Allaire and Jouve 2008) and contact problems (Myśliński 2008). The reader can refer to the comprehensive review in van Dijk *et al*. (2013) for more theoretical details of different LSMs for structural topology optimization.

Density-based methods are the most commonly used topology optimization approaches, such as the popular solid with isotropic material with penalization (SIMP) method. The SIMP method uses continuous design variables for topology optimization, which can be interpreted as material pseudo densities (Bendsøe 1989, Zhou and Rozvany 1991, Mlejnek 1992). The physical justification of the SIMP method was provided by Bendsøe and Sigmund (1999). A popular 99-line topology optimization Matlab code using the SIMP method was developed by Sigmund (2001) for education purposes. As a successor of the 99-line code, a more efficient 88-line Matlab code was also provided by Andreassen *et al*. (2011) with high computational efficiency and alternative filter implements. More details about theory, numerical methods and applications on the SIMP method can be found in (Bendsøe and Sigmund 2004).

As another important branch of topology optimization, evolutionary structural optimization (ESO) (Xie and Steven 1993, 1997, Tanskanen 2002) and its later version bidirectional ESO (BESO) (Da *et al.* 2018c) have shown promising performance when applying to a wide range of structural design problems. ESO-type methods use a simple heuristic scheme to evolve the structural topology towards an optimum by gradually removing redundant or inefficient materials. The BESO method allows not only material removal but also material addition, showing efficient and reliable performance in various design problems (Huang and Xie 2008, 2010, Huang *et al*. 2011, Xia and Breitkopf 2014a,b, 2015b, Huang *et al*. 2015, Vicente *et al*. 2015, Da *et al*. 2017a). The early development of ESO-type methods was summarized by Xie and Steven (Xie and Steven 1997). The development of the BESO method and its various applications up to 2010 can be found in Huang and Xie (2010). A comprehensive review on the BESO method for advanced design of structures and materials was recently presented by Xia *et al*. (2018b).

As an extension to the original BESO method, the author and his collaborators proposed a new evolutionary topology optimization (ETO) method (Da *et al*. 2018c) to design continuum structures, by introducing a sensitivity-based level-set function (LSF). The proposed ETO method identifies the topology far beyond its elements, which does not involve the removal/addition of elements during the optimization process, resulting in a smoothed boundary representation and high robustness. The smooth structural topology has been extended to the robust topology optimization of continuum structures under loading and material uncertainties by Martínez-Frutos and Herrero-Pérez (2018). Inspired by the ETO method, the material removal scheme of evolutionary-type methods has been combined with the LSM to nucleate holes in the structure for optimization design of heat conduction (Xia *et al*. 2018c).

Recently, a new computational framework for structural topology optimization based on the concept of moving morphable components has been proposed (Guo *et al*. 2014). The basic idea of this method is to use a set of deformable components as the basic building block of optimization structures, in order to tailor the structure topology through deformation, merge and overlap operations between components. Therefore, the design variables of the method are reduced during the topology optimization process, and the topological geometries of the structure can be presented explicitly (Zhang *et al*. 2016, Guo *et al*. 2016, Zhang *et al*. 2017).

I.2.2. *Material design and multiscale optimization*

Initially restricted to optimizing the geometry of structures, topology optimization techniques have now been extended to optimizing the topology of the phase within materials, for example in periodic microstructures, to design high performance materials (Sigmund 1994, Sigmund and Torquato 1997, Sigmund 2000, Yi *et al*. 2000, Guest and Prévost 2006, 2007, Wang *et al*. 2014a, Andreassen and Jensen 2014, Chen and Liu 2014, Huang *et al*. 2015), materials with properties not found in nature (e.g. negative Poisson’s ratio, zero compressibility, negative bulk modulus; see Wang *et al*. (2014b), Clausen *et al*. (2015), Da *et al*. (2017b), Noguchi *et al*. (2018)) or complex multi-physics problems (Nanthakumar *et al*. 2016, 2017). These techniques are based on optimizing the homogenized properties of the representative volume element and using numerical solving methods such as finite elements to compute the homogenized properties (Michel *et al*. 1999, Hassani and Hinton 1998a,b, Andreassen and Andreasen 2014), given one geometry of the phases and their microscopic properties, as shown in Figure I.4. A review of topology optimization of microstructures in the linear context can be found in, for example, Cadman *et al*. (2013).

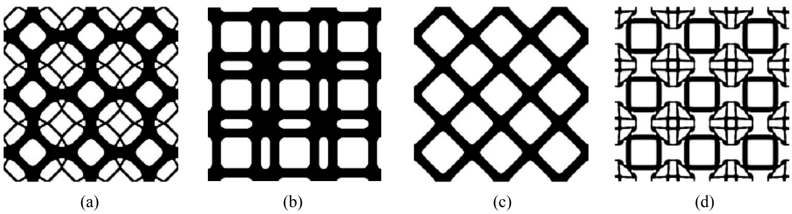


Figure I.4. *Material topologies with extreme elastic modulus and negative Poisson's ratio: (a, b) geometries with maximum bulk modulus, (c) geometry with maximum shear modulus and (d) geometry with negative Poisson's ratio (Da* et al. *2017b)*

Rather than pure material design, material microstructures have also been tailored for a fixed structure (Huang *et al*. 2013) to maximize macroscopic performance under specific boundary conditions, for example structural stiffness (Da *et al*. 2018d). In order to fully release the design freedom within multiscale optimization, Rodrigues *et al*. (2002) first described a hierarchical computational procedure for optimization of material distribution as well as the local material properties of mechanical elements that was later extended to 3D in Coelho *et al*. (2008) and to account for hyperelasticity. With this design strategy, simultaneous structure and materials design has been extensively studied, such as for composite laminate orientations

(Setoodeh *et al.* 2005, 2006, Coelho *et al.* 2015), closed liquid cell materials (Lv *et al.* 2014) or multi-objective functions, for example maximum stiffness and minimum resistance to heat dissipation in de Kruijf *et al.* (2007) or minimum thermal expansion of the surfaces in Deng *et al.* (2013). Extensions to nonlinear materials (Xia and Breitkopf 2014a), multiple-phase materials (Da *et al.* 2017a) and optimization considering uncertainties (Guo *et al.* 2015, Xu *et al.* 2015) have been proposed recently.

In the context of non-separated scales, the effectiveness of the classical homogenization-based multiscale topology optimization framework for periodic lattice structures will be first investigated here in this book. The characteristic dimensions of periodic unit cells in the lattice are comparable with the dimensions of the whole structure such that the two scales cannot be clearly separated. The dimensions of the unit cell range from large to small compared with the dimensions of the whole structure to highlight the size effect. By assuming that the material microstructures are infinitely small, the inverse homogenization designs for macroscopic structural performance were compared with the mono-scale topology optimization framework in Xie *et al.* (2012) and Zuo *et al.* (2013a).

On the other hand, several computational homogenization methods modeling complex heterogeneous media when scales are not separated are available (e.g. gradient models in Peerling *et al.* (1996) and Kouznetsova *et al.* (2002), non-local elasticity theories in Eringen and Edelen (1972) and domain decomposition methods in Ladevèze *et al.* (2001)). Among them, the filter-based non-local homogenization technique developed in Yvonnet and Bonnet (2014a,b) and Tognevi *et al.* (2016) was adopted by Da *et al.* (2018b) to develop a topology optimization procedure for heterogeneous lattice materials in the context of non-separated scales, taking into account the strain gradient effects. The technique generalizes the homogenization theory by replacing spatial averaging operators by linear low-pass filters, and the major advantage is that it can take into account an arbitrary level of strain gradient without higher-order elements, in a classical finite element framework.

In the case of fixed/optimized microscopic periodic cells, multiscale topological design of mesoscopic structures without scale separation is firstly proposed in this book and will be detailed in a later chapter. The idea is to use a computational homogenization method that takes into account the strain gradient effects combined with a topology optimization scheme of mesoscopic structures, allowing the topology optimization problem to be performed on a coarse mesh, instead of using the fully detailed description of the structure for computational saving, as shown in Figure I.5. In addition, other studies, for example Zhang and Sun (2006) and Alexandersen and Lazarov (2015) have also been devoted to the topology optimization of structures in the context of non-separated scales.

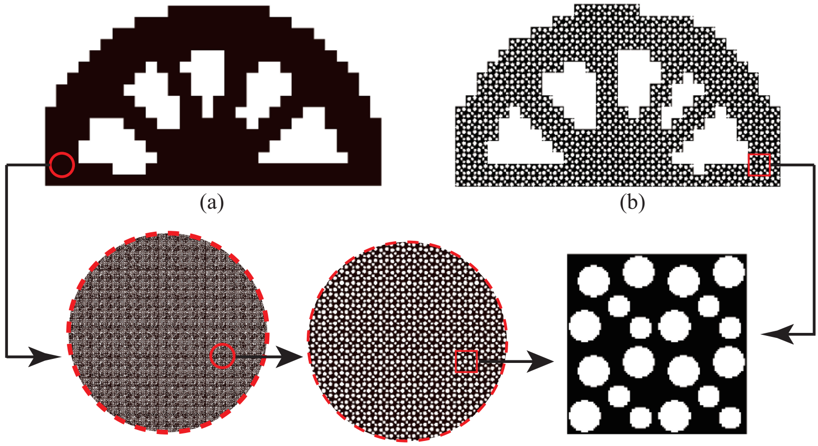


Figure I.5. *Illustration of the two-scale optimized structure composed of the patterned microstructure periodically with (a) scale separation and (b) non-separated scales. For a color version of this figure, see www.iste.co.uk/da/topology.zip*

I.2.3. *Fracture resistance design*

Optimization design of composite materials accounting for fracture resistance has remained relatively unexplored so far, mainly due to the lack of robust numerical methods for simulation of fracture propagation in the presence of complex heterogeneous media and interfaces until recently. In addition, these numerical simulation models should be formulated in a context compatible with topology optimization (e.g. finite elements). Gu *et al*. (2016) used a modified greedy optimization algorithm for composites made up of soft and stiff building blocks to improve material toughness. San and Waisman (2016) explored the optimal location of carbon black particles to maximize the rupture resistance of polymer composites using a genetic algorithm. In a recent work by the author and his coworkers (Xia *et al*. 2018a), topology optimization for maximizing the fracture resistance of quasi-brittle composites was introduced by combining the phase field method and a gradient-based BESO algorithm. However, in the mentioned work, the crack propagation resistance was only evaluated on the basis of phase distribution. In most heterogeneous quasi-brittle materials (e.g. ceramic matrix composites, cementitious materials), the interfacial damage plays a central role in the nucleation and propagation of microcracks (Tvergaard 1993, Lamon *et al*. 2000, Nguyen *et al*. 2016a, Narducci and Pinho 2017). Therefore, we further extended the design framework developed by Xia *et al*. (2018a) in order to define through topology optimization the optimal phase distribution in a quasi-brittle composite with respect to fracture resistance, taking into account crack nucleation in both the matrix and the interfaces, as shown in Figure I.6. To the author's best knowledge, such a study is investigated in this book for the first time.

Simulating interfacial damage and its interaction with matrix crack for complex heterogeneous materials is a highly challenging issue for meshing algorithms. Many numerical methods such as the eXtended Finite Element Method (XFEM) (Moes *et al*. 1999, Sukumar *et al*. 2000), the thick level-set (TLS) method (Bernard *et al*. 2012, Cazes and Moes 2015) and the phase field method (PFM) (Francfort and