Isogeometric topology optimization for computational design of re-entrant and chiral auxetic composites

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Abstract

Auxetic composites, a kind of rationally artificial materials, possess superior multifunctional properties due to a mixture of materials. In this paper, an Isogeometric Topology Optimization (ITO) method is proposed for computational design of both the re-entrant and chiral auxetic composites in both 2D and 3D. The homogenization is numerically implemented using isogeometric analysis (IGA) to predict macroscopic effective properties of microstructures, where the periodic boundary formulation is imposed. An effective Non-Uniform Rational B-splines (NURBS)-based Multi-Material Interpolation (N-MMI) model is applied to compute material properties of all points in composite microstructures, mainly including the Fields of Design Variables (DVFs), Fields of Topology Variables (TVFs), and multi-material interpolation. A unified ITO formulation is developed for 2D and 3D auxetic composites, where an appropriate objective function with a weight parameter is defined to control the generation of different deformation mechanisms. Finally, several numerical examples are performed to demonstrate the effectiveness of the proposed ITO method, and a series of 2D and 3D auxetic composites with the re-entrant and chiral deformation mechanisms are found. The optimized composite structures are simulated using ANSYS to show the auxetic behavior.

Keywords: Auxetic composites; Topology optimization; Isogeometric analysis; Material microstructures; Homogenization

1. Introduction

Auxetic materials are a kind of rationally designed artificial materials, which feature the counterintuitive dilatational behavior \cite{1,2}. That is, contracting laterally if compressed and expanding if stretched laterally. Such materials have attracted enormous attention and gained extensive applications, like sports equipment \cite{3}, textile, aerospace, and defense structures, and body armor \cite{4,5}. It is known that macroscopic effective properties of auxetic materials are mostly on account of the architecture of their material microstructures, rather than the constituent properties of materials. The earlier efforts for the design of auxetic materials are mainly devoted to adjusting

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geometric features of material microstructures, such as sizes and shapes [6–10]. Auxetic materials with many different deformation mechanisms are provided, such as the re-entrant deformation mechanism [8] and the chiral-type [7,9]. For the state-of-the-art of different types of auxetic materials we can refer to [4,5]. Earlier analytical, numerical or experimental methods are developed on the basis of the human intuition and insight to modify the structural sizes or shapes of auxetic materials, which might be a limitation to further find new auxetic materials. Topology optimization [11] is a numerical method to find the optimal material distribution with the expected structural performance, which has been applied to solve several optimization problems [12–17]. Meanwhile, the homogenization theory [18] is proposed to evaluate the macroscopic effective properties of composites using the micro information. An inverse homogenization procedure is developed for the design of material cells with the Negative Poisson Ratios (NPRs) [19] using the topology optimization. Later, this seminal work has been inspired and also extended to find a series of materials with the NPRs [20–28]. For instance, several auxetic material microstructures with many new topologies in 2D were found in [20,22,23], and the optimization of 3D material microstructures with auxetic behavior was addressed in [21,24,26,27]. In order to save the computational cost in the optimization of 3D auxetic material microstructures, several geometric symmetries are pre-defined on the design domain to reduce the possible design space [26,27].

Composite materials have significantly or preferably physical, chemical or mechanical properties [29] if compared to traditional materials. In recent years, the applications of composites, like auxetic composites, have been growing in many engineering fields. A novel concept to develop composite structures with the isotropic NPRs was proposed in [30]. In [31], hybrid materials consisting of auxetic and non-auxetic inclusions were discussed. As far as topology optimization for auxetic composites, a reconciled level set method was applied to optimize the bi-material microstructures with the NPRs [32], where a series of 2D re-entrant auxetic microstructures and only a 3D microstructure were found. Topology optimization for the chiral auxetic composites with the bi-material microstructures in 2D were studied in [33], where the specific initial designs with the chiral features were defined to ensure the form of the chiral deformation mechanism in final designs. To our best knowledge, only a few numbers of works have been performed for auxetic composites, particularly in 3D, which might constrain their further engineering applications. Moreover, a unified topology optimization formulation for the re-entrant and chiral auxetic composites is still in lack.

On the other side, all previous works for auxetic microstructures using topology optimization are based on finite element method (FEM) [34]. However, the deficiencies of FEM significantly affect the effectiveness of topology optimization, such as (1) the finite element mesh cannot exactly capture the structural geometry and (2) the lower-order (C0) continuity of the responses. Isogeometric analysis (IGA) [35,36] is a recently proposed computational approach to unify the Computer-Aided Design (CAD) model with the Computer-Aided Engineering (CAE) model into the same formula. Recently, IGA has attracted much interest among researchers and obtained great developments in many fields [37–40]. The earlier work that introducing the IGA into topology optimization was performed in [41]. IGA for topology optimization with a phase field model was studied for minimizing the compliance in [42]. An isogeometric approach to structural topology optimization was also discussed, where the optimality criterion was used to evolve design variables [43]. Qian [44] addressed the B-spline space for topology optimization with the discussions of the B-spline filter. Recently, the IGA-based Level Set Methods (LSM) for topology optimization have been also performed in [45–47]. Meanwhile, the multiresolution topology optimization using IGA was studied in [48,49]. The IGA-based explicit topology optimization was also addressed in [50–52]. An ITO method with a density distribution function was proposed in [53], and then combined with the homogenization was applied to optimize auxetic metamaterials [54]. The multilevel mesh for ITO to improve the efficiency was discussed in [55]. Recently, the isogeometric shape optimization for auxetic structures with a fixed topology has been studied in [56–58]. For a comprehensive review for the structural design optimization using IGA we can refer to [59]. Hence, how to develop an ITO method for the computational design of 2D and 3D auxetic composites with different deformation features is still a challenging, outstanding and important research topic in the area of structural optimization.

In the current work, the main intention is to develop a unified ITO method for computational design of the re-entrant and chiral auxetic composites in not only 2D, but also 3D cases. Firstly, the homogenization to predict macroscopic effective properties of a composite microstructure is numerically implemented by IGA, shown in Section 2. Secondly, a NURBS-based Multi-Material Interpolation (N-MMI) model is applied to compute material properties in composite microstructures and represent the layout of multiple materials, displayed in Section 3. In
Section 4, an effective and efficient ITO formulation for the re-entrant and chiral auxetic composites in 2D and 3D is defined, where an appropriate objective function with a shift parameter is given. In Section 5, a flowchart of the ITO method for design of auxetic composites is presented. Finally, several 2D and 3D numerical examples are provided to demonstrate the effectiveness and efficiency of the ITO method for computational design of auxetic composites, and the optimized auxetic designs are also simulated in ANSYS to demonstrate the NPR behavior, given in Section 6. Several concluding remarks are provided in Section 7.

2. IGA-based homogenization

The optimization of auxetic composites needs to predict macroscopic effective properties of microstructures using the homogenization, where NURBS is firstly applied to parametrize the geometry and then construct the displacement solution space in IGA.

2.1. NURBS

In the optimization for auxetic composites, the structural design domain is a square in 2D or a cubic in 3D. Here, a cubic is parametrized by the NURBS, as shown in Fig. 1, which consists of the structural geometry in Fig. 1(a), the NURBS solid in Fig. 1(b), the discretized IGA mesh for the cubic in Fig. 1(c), the integration form of the cubic in Fig. 1(d), and the adopted NURBS basis functions in three parametric directions in Fig. 1(e). The parametrized model is constructed by a linear combination of a series of control points with the NURBS basis functions. Given a lattice of control points \( P_{i,j,k} \in \mathbb{R}^3 \), a tensor product NURBS solid \( S(\xi, \eta, \zeta) \) is defined by:

\[
S(\xi, \eta, \zeta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) P_{i,j,k}
\]  

(1)

where \( o - \xi \eta \zeta \) denotes the parametric coordinates for the cubic, and \( R_{i,j,k}^{p,q,r} \) are NURBS basis functions. \( n, m \) and \( l \) indicate the numbers of NURBS basis functions in three parametric directions, respectively. \( p, q \) and \( r \) correspond to polynomial orders of NURBS basis functions, respectively.

\[
R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) = \frac{N_{i,p}(\xi) M_{j,q}(\eta) L_{k,r}(\zeta) \omega_{ijk}}{\sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} N_{i,p}(\xi) M_{j,q}(\eta) L_{k,r}(\zeta) \omega_{ijk}}
\]  

(2)

where \( \omega_{ijk} \) is the positive weight of the \((i, j, k)_{th} \) control point. \( N_{i,p}, M_{j,q} \) and \( L_{k,r} \) are the univariate B-spline basis functions in three parametric directions, respectively, which are defined by the Cox–de-Boor formula [60]. B-spline basis functions \( N_{i,p}(\xi) \) are defined using the formula with a non-decreasing knot vector \( \Xi = \{\xi_1, \xi_2, \ldots, \xi_{n+p+1}\} \) in the parametric space, as:

\[
N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi \leq \xi_{i+1} \\ 0 & \text{otherwise} \end{cases}, \quad p = 0
\]  

(3)

For \( p \geq 1 \), the B-spline basis functions are given as:

\[
N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)
\]  

(4)

It should be noted that the fractions with the form 0/0 in Eq. (1) are equal to zero. Similarly, B-spline basis functions \( M_{j,q} \) and \( L_{k,r} \) are also defined by the Cox–de-Boor formula with the corresponding knot vector \( \mathbb{H} = \{\eta_1, \eta_2, \ldots, \eta_{m+q+1}\} \) and \( \mathcal{Z} = \{\xi_1, \xi_2, \ldots, \xi_{l+r+1}\} \).

2.2. Numerical discretization in IGA

In IGA, NURBS basis functions are applied to construct the approximation space for the unknown structural response. The basic principle is that the continuous solution space is developed by a linear combination of NURBS basis functions and structural responses at control points. The mathematical formula of the solution space is
consistent with Eq. (1), and control coefficients correspond to the responses of control points, rather than the physical
coordinates for the geometrical model, given as:

\[
\mathbf{u}(\xi, \eta, \zeta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} R_{i,j,k}^{p,q,r}(\xi, \eta, \zeta) \mathbf{u}_{i,j,k}
\]

where \( \mathbf{u} \) is the field of structural responses in the design domain, and \( \mathbf{u}_{i,j,k} \) are the responses at control points.

2.3. Homogenization

In the homogenization, two basic requirements should be met: (1) the scales of microstructures are much smaller
than that of the bulk material, and (2) material microstructure, working as a unit cell, is periodically distributed in
the bulk material. As shown in Fig. 3, the bulk material is configured by an identical material microstructure with
two materials (three phases).
For the linearly elastic material, the displacement field \( \mathbf{u}^f (\mathbf{x}) \) at the bulk material can be characterized by the asymptotic expansion theory, expressed as:

\[
\mathbf{u}^f (\mathbf{x}) = \mathbf{u}_0 (\mathbf{x}, y) + \epsilon \mathbf{u}_1 (\mathbf{x}, y) + \epsilon^2 \mathbf{u}_2 (\mathbf{x}, y) + \cdots
\]  

(7)

where \( \epsilon \) is the aspect ratio between the scales of the microstructure and the bulk material, and it is far less than 1. For numerical simplicity, only the first-order variation term is considered, and the final form of the macroscopic effective tensor of the bulk material \( D^H_{ijkl} \) can be expressed by:

\[
D^H_{ijkl} = \frac{1}{|\Omega|} \int_{\Omega} D_{pqrs} (\varepsilon_0^{(ij)} - \varepsilon_{pq}(u^{ij})) (\varepsilon_0^{(kl)} - \varepsilon_{rs}(u^{kl})) \, d\Omega
\]  

(8)

where \( |\Omega| \) is the area (2D) or volume (3D) of the microstructure, and \( D_{pqrs} \) is the locally varying elastic property. \( \varepsilon_0^{(ij)} \) is the linearly independent unit test strain field, containing three components in 2D and six in 3D. \( \varepsilon_{pq}(u^{ij}) \) denotes the unknown strain field in the microstructure, which is solved by the following linear elasticity equilibrium equation with \( y \)-periodic boundary conditions:

\[
\int_{\Omega} D_{pqrs} \varepsilon_{pq}(u^{ij}) \varepsilon_{rs}(\delta u^{ij}) \, d\Omega = \int_{\Omega} D_{pqrs} \varepsilon_0^{(ij)} \varepsilon_{rs}(\delta u^{ij}) \, d\Omega, \quad \forall \delta u \in H_{per}(\Omega, \mathbb{R}^d)
\]  

(9)

where \( \delta u \) is the virtual displacement in material microstructure belonging to the admissible displacement space \( H_{per} \) with \( y \)-periodicity, and \( d \) denotes the dimension of material microstructure.

In the numerical implementation of the homogenization, IGA is applied to calculate the structural responses. Meanwhile, periodic boundary conditions should be imposed on material microstructure to guarantee two basic requirements. In the implementation, an energy-based homogenization method (EBHM) [19] with a periodic boundary formulation is employed. In Eq. (5), the displacement field in material microstructure is approximately
constructed by the displacements at control points with NURBS basis functions. Moreover, the displacement field should satisfy periodic boundary conditions, and a general form is expressed by:

\[
\mathbf{u}_k^+ - \mathbf{u}_k^- = \varepsilon (\mathbf{u}_0) \Delta \mathbf{k}
\]  

(10)

where \( \mathbf{k} \) denotes the normal direction of the structural boundary, and \( \mathbf{u}_k^+ \) indicates the displacements of points at the structural boundary with the normal direction \( \mathbf{k} \), and \( \mathbf{u}_k^- \) corresponds to the displacements of points at the opposite structural boundary. \( \Delta \mathbf{k} \) is the scale of microstructure in the normal direction \( \mathbf{k} \). Hence, control points at the structural boundary should be appropriately classified to develop the periodic boundary conditions, and for the details we can refer to [61] for 2D and [62,63] for 3D.

3. NURBS-based multi-material interpolation (N-MMI) model

The earlier work has been developed for topology optimization of multi-material structures, where many different multi-material topology description models have been developed, such as the mixture rule [64], the DMO scheme [65] and etc. Currently, we have employed the NURBS to construct the multi-material interpolation model, namely the N-MMI model [66]. Firstly, it is assumed that \( \Theta \) distinct materials \((\Theta + 1) \) phases need to be distributed in the design domain. We should introduce \( \Theta \) Fields of Topology Variables (TVFs) \( \phi^\vartheta \) \((\vartheta = 1, 2, \ldots, \Theta) \) to present the overall layout of \( \Theta \) distinct materials. Meanwhile, \( \Theta \) Fields of Design Variables (DVFs) \( \chi^\vartheta \) \((\vartheta = 1, 2, \ldots, \Theta) \) are defined for TVFs in the design domain, and each TVF is defined by a combination of all DVFs.

3.1. The field of design variables (DVF)

The design variables are applied to construct topology variables, and two fundamental requirements should be satisfied in the definition of design variables to ensure the justified topology variables: (1) nonnegativity; (2) strict bounds \([0, 1]\). In Fig. 4, each control point (red dot) is assigned by a control design variable. Before constructing the DVF, the smoothness of control design variables needs to be enhanced to assure the DVF is featured with the desired smoothness. The basic principle is that each design variable is defined by the mean value of all design variables within the local support area. As displayed in Fig. 4, the local support domain of the nodal design variable \( \rho_{i,j,k} \) is the circular area with the radius \( d_m \), given by:

\[
\mathcal{G} (\rho_{i,j,k}) = \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} \psi (\rho_{i,j,k}) \rho_{i,j,k} = \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} \left( \phi (\rho_{i,j,k}) / \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} \tilde{\omega} (\rho_{i,j,k}) \right) \rho_{i,j,k}
\]  

(11)

where \( \mathcal{G} (\rho_{i,j,k}) \) is the smoothed design variable at \((i, j, k)_{th} \) control point, and \( \rho_{i,j,k} \) is the initial design variable. \( N, M \) and \( L \) are the numbers of design variables at the local support area in three parametric directions, respectively. \( \psi (\rho_{i,j,k}) \) is the Shepard function [67] at the current design variable. \( \tilde{\omega} (\rho_{i,j,k}) \) is the weight value of the \((i, j, k)_{th} \) design variable, and the detailed form is given by:

\[
\tilde{\omega} (r) = (1 - r)^6 (35r^2 + 18r + 3), \quad r = d/d_m
\]  

(12)

where \( d \) is the Euclidean distance between the current design variable and other design variables in the local support domain. \( d_m \) is the radius of this area, generally equal to 1.5–2 times the normal scale of IGA elements. For the discussions about the definition of \( d_m \) we can refer to [53].

The DVF is constructed by the linear combination of NURBS basis functions with the smoothed control design variables. Assuming that the DVF in the design domain is denoted by \( \chi \), and the mathematical form is defined as:

\[
\chi (\xi, \eta, \zeta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} R_{i,j,k}^{\rho,q,r} (\xi, \eta, \zeta) \mathcal{G} (\rho_{i,j,k})
\]  

(13)

We can find that Eq. (13) for the DVF is similar to the mathematical form of the NURBS solid in Eq. (1), and the key difference is located at the physical meaning of control coefficient. Meanwhile, the NURBS basis functions make sure the DVF with the nonnegativity and strict bounds \([0, 1]\). Most importantly, the variation diminishing property of NURBS can guarantee the non-oscillatory of the DVF.
3.2. The field of topology variables (TVF)

We introduce $\Theta$ DVFs $\chi^\vartheta$ ($\vartheta = 1, 2, \ldots, \Theta$) to define $\Theta$ TVFs $\phi^\vartheta$ ($\vartheta = 1, 2, \ldots, \Theta$), and each TVF $\phi^\vartheta$ for the layout of a unique material is expressed by the combination of all DVFs. The details of the formula are given as the following:

$$\phi^\vartheta = \prod_{\lambda=1}^{\vartheta} \chi^\lambda \prod_{\lambda=\vartheta+1}^{\Theta} (1 - \chi^\lambda), \quad (\vartheta = 1, 2, \ldots, \Theta)$$

A brief representation for the multi-material topology description is shown in Fig. 5, where each distinct material is plotted with a unique color, namely material 1 with the black, material 2 with the red, material 3 with the green and also a void phase with the white color.

Based on multiple TVFs in Eq. (13), the NURBS-based multi-material interpolation model is defined by a summation of all interpolated functions, each of which is expressed by a TVF interpolated with the physical property.
of the corresponding material, given as:

\[
D = \sum_{\vartheta=1}^{\vartheta} \left( \vartheta^\vartheta \right) D_0^\vartheta = \sum_{\vartheta=1}^{\vartheta} \left( \prod_{\lambda=1}^{\vartheta} (\chi^\lambda)^\vartheta \right) \prod_{\lambda=\vartheta+1}^{\vartheta} (1 - \chi^\lambda)^\vartheta \right) D_0^\vartheta
\]  

(15)

where \( D_0^\vartheta \) is the elastic tensor matrix of the \( \vartheta \)-th distinct material, and \( \gamma \) is the penalty parameter. The key ingredient of the N-MMI model is the definition of two kinds of variables, and they are not coupled into a unified symbol and will be advanced in a serial mechanism. Hence, the N-MMI model can exhibit some positive features: (1) All TVFs with the sufficient smoothness and continuity are applied to represent the layouts of all materials, rather than a discrete form with a series of element densities in spatial. (2) Each TVF can exactly capture the layout of a unique material. (3) The combination of all DVFs for the expression of the TVF can ensure no overlaps between multiple materials and no redundant phases in the design domain, and there is no need to introduce the additional constraints for the variables. (4) The explicit mathematical formula offers more benefits for the latter sensitivity analysis in the formulation.

4. Isogeometric topology optimization (ITO) for auxetic composites

4.1. ITO formulation

It is known that the physical meaning of the Poisson’s ratio corresponds to the deformation mechanism of the bulk material, which is defined by the aspect ratio of the transverse contraction strain to the longitudinal extension strain in the direction of stretching force. In the previous works for the design of auxetic materials, several objective functions are defined to generate material microstructures with the auxetic behavior, such as the minimization of the weighted square difference between the effective elastic tensor and the expected elastic tensor [21,23], the minimization of a combination of the effective elastic tensor [54,61]. Generally speaking, the latter form of the definition is more stable and efficient in the optimization of auxetic materials with the NPRs. In the current work, the key intention is to develop an ITO method for computational design of auxetic composites by virtue of the superior features from different materials, and a combination of the homogenized elastic tensor of composite microstructure is applied to define the objective function, and the details of the ITO formulation are expressed by:

\[
\text{Find: } \rho^\vartheta \left\{ \rho^\vartheta_{i,j}, \rho^\vartheta_{i,j,k} \right\}
\]

\[
\text{Min: } J (u, \varphi) = -\beta \left\{ \sum_{i,j=1,i=j}^{d} D_{ii,jj}^H (u, \varphi (\rho^\vartheta)) \right\} + \left\{ \sum_{i,j=1,i\neq j}^{d} D_{ii,jj}^H (u, \varphi (\rho^\vartheta)) \right\}
\]

\[
\text{S.t.} \left\{ \begin{array}{l}
\{ a (u, \delta u) = l (\delta u), \quad \forall \delta u \in H_{\text{per}} (\Omega, \mathbb{R}^d) \\
G_v^\vartheta = \frac{1}{|\Omega|} \int_{\Omega} \phi^\vartheta \nu_{0d} \, d\Omega - V_0^\vartheta \leq 0, \quad (\vartheta = 1, 2, \ldots, \Theta) \\
0 < \rho_{\text{min}} \leq \rho^\vartheta \leq 1 \\
\vartheta = 1, 2, \ldots, \Theta; \ i = 1, 2, \ldots, m; \ j = 1, 2, \ldots, n; \ k = 1, 2, \ldots, l
\end{array} \right.
\]

where \( \rho^\vartheta \) denotes control design variables of the \( \vartheta \)-th set, including \( \rho^\vartheta_{i,j} \) in 2D and \( \rho^\vartheta_{i,j,k} \) in 3D. \( J \) is the objective function defined by the combination of the homogenized elastic tensor, where \( \beta \) is a weight parameter. It can be found that the optimizer intends to increase the first term and decrease the second term during the optimization, so that the objective function can arrive at the minimal. As discussed in [19,54,61], the decrease of second term can push its value larger than 0 in the optimization, namely \( D_{ii,jj}^H < 0 (i \neq j) \), which facilitates the form of the mechanism-type features in composite microstructures. The mechanism-type distribution can be beneficial to the generation of the auxetic behavior in the topology. Meanwhile, the increase of the first term can push its value smaller than 0 in the optimization, namely \( D_{ii,jj}^H > 0 (i = j) \). Hence, the definition of the objective function can make the diagonal terms and off-diagonal components with the opposite sign, so that the auxetic composite microstructures can be found using the ITO method. \( d \) is the spatial dimension of composites. \( G_v^\vartheta \) is the volume constraint for the \( \vartheta \)-th distinct material, where \( V_0^\vartheta \) is the maximum material consumption and \( \nu_{0d} \) is the volume fraction of solids. We
can find that all volume constraints have the separable and linear form with respect to TVFs. $\phi^\delta$ is the TVF to show $\hat{\theta}_n$ unique material, defined in Eq. (14). $u$ is the displacement field in composite microstructure, which should meet the periodic boundary conditions in Eq. (10). $\delta u$ is the virtual displacement field in the admissible space $H_{\text{per}}$ with $y$-periodicity, which is calculated by the linearly elastic equilibrium equation. $a$ and $l$ are the bilinear energy function and the linear load function, respectively, given as:

$$\begin{aligned}
a (u, \delta u) &= \int_{\Omega} D \left( \phi \left( \rho^\theta \right) \right) \varepsilon (u) \varepsilon (\delta u) \, d\Omega \\
l (\delta u) &= \int_{\Omega} D \left( \phi \left( \rho^\theta \right) \right) \varepsilon^{0\varepsilon} (\delta u) \, d\Omega
\end{aligned}$$

(17)

where $D$ is the elastic tensor of composites defined by the N-MMI model.

### 4.2. Design sensitivity analysis

In Eq. (16), the ITO formulation is developed for the optimization of auxetic composites. We firstly derive the first-order derivative of the objective function with respect to TVFs $\phi^\delta$, expressed by:

$$\frac{\partial J}{\partial \phi^\delta} = -\beta \left\{ \sum_{i,j,i=L}^d \frac{\partial D_{ij}^H (u, \phi \left( \rho^\theta \right))}{\partial \phi^\delta} \right\} + \left\{ \sum_{i,j,i=L, i \neq j}^d \frac{\partial D_{ij}^H (u, \phi \left( \rho^\theta \right))}{\partial \phi^\delta} \right\}, \quad (\hat{\theta} = 1, 2, \ldots, \Theta)$$

(18)

It can be seen that the first-order derivative of the objective function with respect to TVFs mainly relies on the derivatives of the effective elastic tensor $D_{ij}^H$ with respect to TVFs $\phi^\delta$. For the detailed derivations for the derivatives of the effective stiffness tensor we can refer to [23,33], and the final form is expressed by:

$$\frac{\partial D_{ij}^H}{\partial \phi^\delta} = \frac{1}{|\Omega|} \int_{\Omega} \gamma \left( \phi^\delta \right)^{\gamma-1} D_{\theta, pqrs} \left( \varepsilon_{pq} - \varepsilon_{pq} \left( u^{ij} \right) \right) \left( \varepsilon_{rs} - \varepsilon_{rs} \left( u^{ij} \right) \right) \, d\Omega$$

(19)

As defined in Section 3, $\phi^\delta$ is defined by a combination of all DVFs. Each DVF is constructed by NURBS basis functions with control design variables $\rho^\theta$. we can derive the first-order derivative of the TVF $\phi^\delta$ with respect to the DVF $\chi^\theta$, given as:

$$\frac{\partial \phi^\delta}{\partial \chi^\theta} = \begin{cases} \prod_{\lambda=1, \lambda \neq \theta} \varepsilon (\chi^\lambda) \prod_{\lambda=\theta} (1 - \chi^\lambda) & \text{if } \theta \leq \hat{\theta} \\
- \prod_{\lambda=1} \varepsilon (\chi^\lambda) \prod_{\lambda=\theta+1, \lambda \neq \theta} (1 - \chi^\lambda) & \text{if } \theta > \hat{\theta} \end{cases}, \quad (\theta = 1, 2, \ldots, \Theta)$$

(20)

Then, the derivative of DVF with respect to control design variables $\rho^\theta$ can be achieved by consecutively differentiating Eqs. (13) and (11), and the detailed form with control design variables $\rho^\theta_{i,j,k}$ is given by:

$$\frac{\partial \chi^\theta}{\partial \rho^\theta_{i,j,k}} = \frac{\partial \chi^\theta}{\partial G^\theta} \frac{\partial G^\theta}{\partial \rho^\theta_{i,j,k}} = R_{i,j,k}^{\rho,q,r} (\xi, \eta, \zeta) \psi \left( \rho^\theta_{i,j,k} \right)$$

(21)

where $R_{i,j,k}^{\rho,q,r} (\xi, \eta, \zeta)$ is the NURBS basis function at the computational point $(\xi, \eta, \zeta)$. $\psi \left( \rho^\theta_{i,j,k} \right)$ is the Shepard function at the control point $(i, j, k)$. It is noted that the above computational point $(\xi, \eta, \zeta)$ is different from the control point $(i, j, k)$. The former corresponds to Gauss quadrature points, which lies in the design domain. However, the lattice of control points forms a polygon in spatial, which contains the structural geometry. Some of control points are not necessary at the structural geometry. Finally, the derivatives of the homogenized elastic tensor with respect to control design variables can be derived by Eqs. (19)–(21), and the final form is explicitly expressed.
as:
\[
\frac{\partial D_{\acute{H}}^{\hat{\varphi}}_{i,j,k}}{\partial \rho^0_{i,j,k}} = \sum_{\hat{\varphi}} \frac{\partial D_{\acute{H}}^{\hat{\varphi}}_{i,j,k}}{\partial \phi^\hat{\varphi}} \frac{\partial \varphi^\hat{\varphi}}{\partial \rho^0_{i,j,k}} = \cdots
\]

\[
\sum_{\hat{\varphi}=1}^{\varphi} \left\{ \begin{array}{l}
\frac{1}{|\Omega|} \int_{\Omega} \left( \gamma (\chi^0)^{\hat{\varphi}-1} \prod_{\lambda=1, \lambda \neq \hat{\varphi}}^{\hat{\varphi}} (1 - \chi^\lambda) \right) D_{0,m,n,p,q,r} \cdots \right. \\
\left. \frac{R^{p,q,r}_{i,j,k} (\xi, \eta, \zeta) \psi (\rho^0_{i,j,k}) \left( \begin{array}{c} 0_i \hspace{1cm} - \epsilon_{pq} \left( u^{ii} \right) \\
\epsilon_{rs} \left( u^{ij} \right) \end{array} \right) \right) d\Omega \right\} \quad \text{if } \varphi \leq \hat{\varphi}
\end{array} \right. \\
\right\}
\]

Similarly, the derivatives of the objective and constraint functions are strongly dependent on the NURBS basis functions at Gauss quadrature points and the Shepard function at control points. The NURBS basis functions and Shepard function only depend on the spatial locations of the points and keep unchanged during the optimization. Hence, they can be pre-stored without using additional storage space, and the sensitivity analysis of the objective function is cost-effective. The method of moving asymptotes (MMA) \[68\] is used to evolve design variables in next numerical examples.

An example of the design domain with two 1D TVFs is shown in Fig. 6, and the definition of each TVF is applied to represent the topology of one material. In Fig. 6, TVF1 to represent the layout of M1 material and TVF2 to display the M2 material distribution are defined. The materials interface is displayed in point A. In terms of the derivative of the objective function, we can find that each TVF to present the layout of a distinct material is a continuous function in the design domain, and the objective function is derivative with respect to each TVF. Meanwhile, as already studied in Section 3.2 for the N-MMI model, we can achieve that the TVFs using the combination of the TVFs can ensure no overlap areas in the representation of the materials, namely each designable point only containing one distinct material or void. Thus, we can confirm that the discontinuity feature does not occur in both the TVFs and the derivatives of the objective function with respect to the TVFs. As displayed in Fig. 6, two TVFs have the cross point A at the value equal to 0.5. The iso-value (0.5) of the TVFs represents the structural boundaries, which does not introduce the overlap in the representation of the solid materials using TVFs. Hence, we can conclude that the materials interface stemming from the cross point has no influence on the numerical stability in the optimization.

5. Numerical implementations

As shown in Fig. 7, a flowchart in detail of the ITO formulation for the optimization of auxetic composites is provided. The key steps of the optimization are involved into the following components: the geometry parametrization and then discretization in Sections 2.1 and 2.2, respectively, the construction of the DVFs and
TVFs for multiple materials in Section 3, the homogenization to predict the effective elastic tensor in Section 2.3, the calculation of the objective function and volume fractions in Section 4.1, the sensitivity analysis and the evolving of DVFs and TVFs.

6. Numerical examples

In this section, several numerical examples are provided to demonstrate the effectiveness and efficiency of the ITO method for auxetic composites. Firstly, the discussions of 2D auxetic composites with two different materials are performed to present the basic features of the ITO method, and the shift parameter to control the deformation mechanism is adjusted to achieve several types of auxetic composites. Secondly, the ITO method is applied to perform the optimization of 3D auxetic composites to search for the novel 3D auxetic composite microstructures.
Table 1

<table>
<thead>
<tr>
<th>$i$</th>
<th>Materials</th>
<th>Young's modulus: $E_i^0$</th>
<th>Poisson’s ratio $v$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M1</td>
<td>10</td>
<td>0.3</td>
</tr>
<tr>
<td>2</td>
<td>M2</td>
<td>5</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Fig. 8. Initial designs of control design variables, DVFs and TVFs for two materials, respectively.

with two types of deformation mechanisms. Finally, the topologically-optimized 2D and 3D auxetic composite structures are also simulated in the software ANSYS to show their auxetic behavior. In the numerical analysis, $3 \times 3$ (2D) or $3 \times 3 \times 3$ (3D) Gauss quadrature points are chosen in each IGA element. The dimensions of microstructures in all directions are set to be 1. The penalty parameter $\gamma$ in Eq. (15) is set to be 3. Two “virtual” isotropic solid materials will be considered in next examples, and the related details are provided in Table 1.

6.1. 2D auxetic composites

The optimization of 2D auxetic composites with the re-entrant and chiral deformation mechanisms will be discussed in Sections 6.1.1 and 6.1.2, respectively. In terms of the design of 2D auxetic composites, the design domain corresponds to a square with the normal scales 1 $\times$ 1 in spatial. The NURBS surface is employed to parametrize the design domain, where the quadratic basis functions are chosen and the knot vectors are set as: $\Xi = H = \{0, 0, 0, 0.01, \ldots, 0.99, 1, 1, 1\}$. The corresponding IGA mesh for the design domain has $100 \times 100$ elements, and $102 \times 102$ (10 404) control points are contained. Two distinct materials (M1 and M2) pre-defined in Table 1 will be considered in the next optimization. The allowable volume fractions $V_0^\theta (\hat{\vartheta} = 1, 2)$ for M1 and M2 materials are defined as 20% and 20%, respectively. As already pointed out in Section 3, two DVFs $\chi^\vartheta (\vartheta = 1, 2)$ and two TVFs $\phi^\vartheta (\vartheta = 1, 2)$ should be defined in the optimization of auxetic composites with two unique materials. In the construction of DVFs, two sets of control design variables $\rho^\vartheta (\vartheta = 1, 2)$ are introduced for the definition of two DVFs, respectively. As displayed in Fig. 8(a1) and (a2), the initial values of two sets of control design variables are provided, and the corresponding two DVFs in the design domain are shown in Fig. 8(b1) and (b2), and the initial designs of two TVFs for the overall layout of two unique materials are displayed in Fig. 8(c1) and (c2). It should be noted that the height direction denotes the values of variables.

6.1.1. 2D auxetic composite with the re-entrant deformation mechanism

In [54], the effect of the shift parameter $\beta$ in the objective function on the design of auxetic metamaterials has been studied. Here, in order to obtain 2D auxetic composite with the re-entrant deformation mechanism, the constant parameter $\beta$ is defined to be 0.03 to obtain the re-entrant auxetic composites with the same NPRs in different normal directions.
The optimized designs of two TVFs $\phi^\vartheta$ ($\vartheta = 1, 2$) to present the distributions of $\text{M1}$ and $\text{M2}$ materials in the design domain are shown in Fig. 9(a1) and (a2), respectively. As we can find, the optimized TVFs for two distinct materials are featured with the desired smoothness and continuity, even if the initial designs in Fig. 8(c1) and (c2) still have dramatic changes from the lower to upper bounds. According to the N-MMI model, each TVF is a combination of all DVFs, which can be viewed as a density distribution function to represent the layout of the distinct material. In the construction of the DVF and TVF, the Shepard function can guarantee the smoothness of DVFs and NURBS basis functions can assure the continuity of DVFs. The positive features can offer more benefits for the representation of the topology [53,54]. Additionally, the values of the optimized TVFs for $\text{M1}$ and $\text{M2}$ materials are mostly identical to 0 or 1, and only a narrow area is existed for the changing from 0 to 1 in a smooth and continuous manner.

Here, a simple but efficient heuristic criterion is introduced to define the structural topology, given in Eq. (24). As we can see, structural boundaries of the optimized composite microstructure are expressed by the iso-contour $\phi_c$ of $\phi^\vartheta$ with the values higher than $\phi_c$, denotes solids in the topology, and the values smaller than $\phi_c$ describes the voids. However, it should be noted that the current heuristic criterion is just a post-definition scheme to define the topology for the composite microstructure using the optimized TVFs $\phi^\vartheta$ ($\vartheta = 1, 2$). The key characteristic of the ITO method for auxetic composites is to optimize the TVFs for the distributions of materials in the design domain.

$$
\begin{align*}
0 &< \phi (\xi, \eta) < \phi_c & \text{void} \\
\phi (\xi, \eta) &= \phi_c & \text{boundary} \\
\phi_c < \phi (\xi, \eta) &\leq 1 & \text{solid}
\end{align*}
$$

In the current work, the constant $\phi_c$ is set as 0.5, due to a basic fact that the values of $\phi^\vartheta$ ($\vartheta = 1, 2$) in the design domain are mostly identical to 0 or 1, nearly ranging in two intervals $[0, 0.1]$ and $[0.9, 1]$. Moreover, in the N-MMI model, the constant 0.5 can ensure no overlaps between different materials and no redundant phases. For example, if the constant $\phi_c$ is equal to 0.2, it means that densities at structural boundaries of $\text{M1}$ and $\text{M2}$ materials are both equal to 0.2, and the summation of them is equal to 0.4, which cannot satisfy the summation of the densities of all materials in each designable point that is equal to 1. Hence, the constant $\phi_c$ must be equal to 0.5 to guarantee the reasonable physical meanings of the N-MMI model. As shown in Table 2, the optimized topologies for two materials in the design domain are listed, namely the topologies of $\text{M1}$ and $\text{M2}$ materials, the topology of auxetic composite microstructure, the homogenized elastic tensor and the NPR value. Based on the optimized topology, we can find that the re-entrant mechanism is formed by $\text{M1}$ and $\text{M2}$ materials, which can generate the auxetic behavior with the imposing of a load on auxetic composite microstructure. Additionally, a representation for the re-entrant auxetic composite is also shown in Fig. 10, where $5 \times 5$ repetitive microstructures briefly describe the bulk auxetic composite.

As already discussed in the above paragraph, the iso-contour of TVFs is applied to represent the structural boundaries, where the iso-value is equal to 0.5. The TVFs correspond to the NURBS response surface to represent the topologies of materials. Hence, the iso-contour of the TVFs in a normal direction correspond to the NURBS curve. The structural boundaries can be exactly represented by the NURBS curve, shown in Fig. 11. According to the results shown in Figs. 10 and 11, we can easily found that the topology of the auxetic composite microstructure has the smooth structural boundaries and distinct interfaces between the solids and voids, which might lower the numerical difficulties for the latter manufacturing phase.
Finally, the convergent histories of the objective function and volume fractions of two materials are shown in Fig. 12. As we can see, the initial iterative steps (nearly 30) have the dramatic changes, mainly because the volume fractions of \( M_1 \) and \( M_2 \) materials in the initial designs are not equal to the prescribed values. After 30 steps, the optimization of auxetic composites is very stable and quickly arrives at the pre-defined convergent condition that the optimization will be terminated within 101 iterations. Although the objective function is still decreasing in the final steps, the TVFs of \( M_1 \) and \( M_2 \) materials keep stable with only a few changes to adjust the structural boundaries. As shown in Fig. 13, the intermediate results of the TVFs are provided to show this feature. Hence, it is enough to achieve the desired auxetic composite microstructures with the novel topology in 101 iterations.
Fig. 12. Convergent histories of the objective function and volume fractions.

Fig. 13. Intermediate results of TVFs $\phi^\theta$ ($\theta = 1, 2$).
6.1.2. Discussions of the weight parameter

As addressed in [54], the weight parameter has the capability to control the generation of the deformation mechanism on the optimization of auxetic metamaterials. In the current section, we aim to adjust the value of weight parameter $\beta$ to generate auxetic composite microstructures with different deformation features and also discuss the effect on the optimization of auxetic composites with two distinct materials. Ten cases are performed, where weight parameters are defined as 0.003, 0.015, 0.03, 0.05, 0.08, 0.1, 0.15, 0.2, 0.25, 0.3. Other design parameters keep consistent with the above example, for instance the NURBS details, the maximum volume fraction for two materials, the initial designs etc.

The optimized auxetic composite microstructures in ten cases are shown in Fig. 14, also with the minimum NPRs in two normal directions. Firstly, the values of the NPRs in ten cases are increased when the weight parameter is varied from 0.003 to 0.3. That is, the auxetic behavior in microstructures becomes smaller and smaller in ten cases. The influence of weight parameter on the optimization of auxetic composites has the same varied trend compared to its effect on the optimization of auxetic metamaterials. Secondly, when the weight parameter is changed from 0.03 to 0.25, the optimized auxetic composite microstructures in seven cases have the same NPRs in two normal directions. If the weight parameter is decreased, the optimizer tends to minimize the NPR in one normal direction, and the optimized auxetic composite microstructure is the orthotropic. In the last case with weight parameter 0.3, the obtained microstructure is not featured with the auxetic behavior. Hence, the numerical results coincide with the theoretical analysis about the effect of the objective function on the optimization, and weight parameter is a scaling factor to claim the importance of different terms in the objective function.

Moreover, we also perform one case with an extremely low value of weight parameter, namely 0.0001. As shown in Fig. 15, the optimized TVFs $\phi^\theta$ ($\theta = 1, 2$) for the distributions of $M_1$ and $M_2$ materials, as well as the combined TVFs for the overall distribution are provided. Similar to the example in Section 6.1.1, the optimized TVFs are also featured with sufficient smoothness and continuity, which can offer more benefits for the latter representation of the topologies in the design domain. Moreover, the values of the optimized TVFs also mostly approach the lower or upper bounds only with a narrow area for the transition between 0 and 1. Hence, the heuristic but efficient scheme to define the structural topology in Eq. (24) is still adopted here, where the constant $\phi_c$ is still set as 0.5 to guarantee the reasonable physical meanings of the N-MMI model for the distribution of multiple materials.

The optimized numerical results in this case are listed in Table 3, including the final topologies of $M_1$ and $M_2$ materials, the topology of the auxetic composite microstructure, its homogenized elastic tensor and the corresponding NPR values in two normal directions. We can easily find that $M_1$ and $M_2$ materials can be
appropriately distributed in the final topology to form the chiral deformation mechanism. In order to clearly demonstrate the chiral feature, the corresponding auxetic composite with $5 \times 5$ microstructures is shown in Fig. 16(d). As we can see, the chiral auxetic behavior is generated by a combination of materials in four corners of the optimized composite microstructure.

According to the above eleven cases, only a shift parameter is adjusted in the optimization to obtain auxetic composites. Moreover, there is no need to define the specific initial designs before the optimization to form the corresponding deformation mechanism [33]. Hence, it can be concluded that the ITO method has the superior capability to optimize the 2D auxetic composites with not only the re-entrant feature, but also the chiral deformation mechanism. Additionally, it should be noted that the values, like 0.0001, 0.03, 0.25 and 0.3, are not the changing bounds of auxetic composite microstructure with different structural mechanisms. In all numerical examples, the effect of weight parameter on the optimization of composite microstructure can be only discussed in a qualitative analysis, not in a quantitative test with the definitive values. In fact, these values can provide a reasonable direction for the optimization of auxetic composite microstructures with different deformation features, which can perfectly satisfy the key requirements of the ITO method on seeking for the novel auxetic composites.

![Fig. 15. The optimized designs of $\phi^\theta$ ($\theta = 1, 2$).](image)

### Table 3
The optimized 2D chiral auxetic composite microstructure.

<table>
<thead>
<tr>
<th>M1 material</th>
<th>M2 material</th>
<th>The topology</th>
<th>D$^H$</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Image" /></td>
<td><img src="image" alt="Image" /></td>
<td><img src="image" alt="Image" /></td>
<td><img src="image" alt="Image" /></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$u_{11}$ $u_{12}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.514 $-0.354$ 0.0122</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$-0.354$ 0.535 $-0.0114$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0122 $-0.0114$ 0.0128</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>$u_{11}$ $u_{12}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-0.689 $-0.662$</td>
</tr>
</tbody>
</table>
6.2. 3D auxetic composites

In this section, the optimization of 3D auxetic composites with different deformation features is studied. M1 and M2 materials are available in the optimization, and the corresponding volume fractions are defined as 25% and 20%, respectively. In order to clearly present the topology in 3D cases, the red and green colors are applied to show M1 and M2 materials, respectively. As far as the optimization of 3D auxetic composite microstructure, the design domain is a cubic with the size $1 \times 1 \times 1$, shown in Fig. 17(a). The NURBS solid is used to parametrize the design domain, and the quadratic NURBS basis functions are used and the knot vectors are set as: $\Xi = \Xi = Z = \{0, 0, 0, 0.0417, \ldots, 0.9583, 1, 1, 1\}$. The NURBS solid and IGA mesh of the cubic are shown in Fig. 17(b) and (c), respectively. The IGA mesh for the design domain has $24 \times 24 \times 24$ elements, and $26 \times 26 \times 26$ control points are included in NURBS solid. In IGA, an element will contain $3 \times 3 \times 3$ Gauss quadrature points, and the total number of Gauss quadrature points is equal to $72 \times 72 \times 72$. As given in Section 3, the corresponding control design variables $\rho_\theta$ ($\theta = 1, 2$), two DVFs $\chi_\theta$ and two TVFs $\phi_\theta$ for M1 and M2 materials are 4D function, and it is hard to suitably display the 4D function in 3D space. Hence, we only display the corresponding iso-surfaces.

As shown in Fig. 18, three different initial designs of two sets of control design variables $\rho_\theta$ ($\theta = 1, 2$), two DVFs and two TVFs are defined to seek for a series of novel auxetic composites, where the corresponding iso-values are also provided. The initial values of control design variables are mostly equal to 0.5, and with several homogeneously distributed holes. In three initial designs, the distributed forms of the holes in the design domain are different. Meanwhile, it should be noted that TVFs are calculated by Eq. (14), and mostly equal to 0.25. Hence, the iso-surface (0.25) of TVFs can clearly describe the initial designs. It should be noted that the iso-value of TVFs...
for the latter representation of the topology is still equal to 0.5 to ensure the reasonable physical meanings of the N-MMI model.

6.2.1. 3D auxetic composite with the re-entrant deformation mechanism

The weight parameter $\beta$ is defined to be 0.03 in the first case to obtain 3D re-entrant auxetic composite microstructures with the same NPRs in two normal directions. The initial design 1, shown in Fig. 18(a), is used in case 1. The optimized 3D auxetic composite microstructure with $\text{M1}$ and $\text{M2}$ materials is shown in Fig. 19, including the topologies of $\text{M1}$ and $\text{M2}$ materials, the cross-sectional views of them, the final topology of the 3D auxetic composite microstructure and its corresponding cross-sectional view. As we can see, the optimized 3D auxetic composite microstructure is featured with the smooth structural boundaries and distinct interfaces between the solids and voids in the topology. Meanwhile, $3 \times 3 \times 3$ composite material microstructures briefly represent a 3D auxetic composite with the periodicity of microstructures, shown in Fig. 20(a). In order to present the interior information, its cross-sectional view is also displayed in Fig. 20(b). According to the details of the 3D auxetic composite microstructure shown in Figs. 19 and 20, the re-entrant deformation mechanism can be easily observed from the distribution of $\text{M1}$ material (red color in Figs. 19 and 20). The corresponding homogenized elastic tensor of the optimized microstructure is listed in Table 4, and we can find the NPRs in three normal directions are all equal to $-0.0852$. Hence, the optimized 3D composite microstructure shown in Figs. 19 and 20 is also featured with the auxetic behavior based on the quantitative computation.

Meanwhile, we also provide the convergent histories of the objective function and volume fractions of two materials, shown in Fig. 21. As we can see, the former iterations (nearly 40th) of the objective function and constraint functions have the dramatic changes. The objective value gradually decreases with the increasing of the volume fraction of $\text{M1}$ material, until the auxetic behavior emerges in the topology. Later, the volume fraction of $\text{M1}$ material quickly arrives at the pre-defined value, and the latter steps (from 41th to 120th step) gradually adjust the obtained topology in 40th step to meet the volume constraint and simultaneously ensure the optimized composite microstructure is featured with the auxetic behavior. Hence, the optimization of the 3D auxetic composite...
The optimized topology of 3D auxetic composite microstructure No.1 with two materials. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 19. The optimized topology of 3D auxetic composite microstructure No.1 with two materials. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The microstructure is more difficult than 2D case, particularly in the former iterations, mainly due to the increasing number of design freedoms in 3D problem. In the initial iterations of the 3D case, we relax the volume constraints of M1 and M2 materials, so that the optimizer can easily seek for the topology with the auxetic behavior. After the auxetic microstructure is achieved, the latter iterations will be performed to maintain volume constraints. Hence, the developed ITO method has the effectiveness to seek for the novel auxetic composite microstructures. Meanwhile, we can see that the optimized 3D auxetic composite microstructure has the lower auxetic behavior due to the NPRs only equal to \(-0.0852\). The main cause is that the defined objective function can only offer an appropriate direction that the optimizer can seek for the topology with the auxetic behavior. However, it cannot determine the final values of the NPRs in three normal directions. It is noted that this characteristic has a negligible influence on the effectiveness of the ITO method on the design of auxetic composites, due to the fact that the main intention is to seek for the novel topologies of 3D auxetic microstructures. We can use the shape optimization or size optimization to adjust the NPRs of the optimized microstructures in a fixed topology, shown in [22,56,57].

Additionally, it is known that the micro-structured materials design is extensively dependent on the design parameters, like the initial design of the parameters in the optimization and etc., due to the non-uniqueness of the micro-architected design [19,61,62]. Here, in order to seek for many novel 3D auxetic composites with the re-entrant deformation mechanism, we have performed other two cases based on the initial design 2 and 3, shown in Fig. 18(b) and (c), respectively. The optimized 3D auxetic composite microstructures in two cases are presented in Figs. 22–25, respectively, also including the topologies of different materials and their corresponding cross-sectional views.

As shown in Figs. 23 and 25, the optimized auxetic composites No. 2 and 3 with a periodic distribution of $3 \times 3 \times 3$ microstructures are also provided. The corresponding homogenized elastic tensors of two auxetic composite microstructures are also listed in Table 4, and the NPRs of two auxetic composites are equal to \(-0.0782\) and \(-0.0766\), respectively. According to the optimized auxetic composite microstructures, the final topologies in two cases have the auxetic deformation mechanisms.
6.2.2. 3D auxetic composite with the chiral deformation mechanism

As far as the 3D auxetic composite microstructures with the chiral deformation mechanism, the constant parameter $\beta$ is defined to be 0.0001 in the objective function. This case will be performed subject to the initial design 1. The optimized numerical results of this case are displayed in Figs. 26 and 27, also including the topologies of two materials and their cross-sectional views, the topology of 3D microstructure and its cross-sectional view. It can be easily seen that $\text{M2}$ material is formed into the structural member with the chiral deformation mechanism in the final topology. The corresponding homogenized elastic tensor is listed in Table 5. Based on its value, we can easily find that the optimized auxetic composite microstructure No.4 is anisotropic, where the NPRs in three normal directions have different values.

Finally, we also provide the 2D cross-sectional views of auxetic composite microstructures No.1 to No.4, displayed in Fig. 28. As we can see, auxetic composites No.1 to No.3 can be classified into a same branch, where
the auxetic behavior stems from the re-entrant deformation. However, auxetic composite No.4 has two deformation features, where M1 material is formed into the re-entrant structural member and the chiral deformation mechanism is generated by M2 material. Hence, the auxetic behavior of auxetic composite No. 4 originates from a combination of the re-entrant and chiral deformation mechanisms (see Fig. 27).

Fig. 22. The optimized topology of 3D auxetic composite microstructure No.2 with two materials.

(a1, a2 and a3) The topologies of M1 and M2 materials, and the final topology respectively.

(b1, b2 and b3) Cross-sectional views of (a1, a2 and a3), respectively.

Fig. 23. The details of the 3D auxetic composite No.2 with $3 \times 3 \times 3$ microstructures.

(a) The 3D auxetic composite

(b) Cross-sectional view of (a)
6.3. Simulating validation based on ANSYS

In this section, the topologically-optimized auxetic composites in 2D and 3D are both simulated to validate the auxetic behavior using the software ANSYS.
Table 4
Homogenized elastic tensors of auxetic composites No.1 to No.3.

<table>
<thead>
<tr>
<th>3D Auxetic composite No. 1</th>
<th>3D Auxetic composite No. 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3192 −0.0272 −0.0272 0 0 0</td>
<td>0.422 −0.033 −0.033 0 0 0</td>
</tr>
<tr>
<td>−0.0272 0.3192 −0.0272 0 0 0</td>
<td>−0.033 0.422 −0.033 0 0 0</td>
</tr>
<tr>
<td>−0.0272 −0.0272 0.3192 0 0 0</td>
<td>−0.033 −0.033 0.422 0 0 0</td>
</tr>
<tr>
<td>0 0 0 0 0.024 0 0</td>
<td>0 0 0 0 0.034 0 0</td>
</tr>
<tr>
<td>0 0 0 0 0 0.024 0</td>
<td>0 0 0 0 0 0.034 0</td>
</tr>
<tr>
<td>0 0 0 0 0 0 0.024</td>
<td>0 0 0 0 0 0 0.034</td>
</tr>
</tbody>
</table>

3D Auxetic composite No. 3

| 0.496 −0.038 −0.038 0 0 0 | 0.422 −0.033 −0.033 0 0 0 |
| −0.038 0.496 −0.038 0 0 0 | −0.033 0.422 −0.033 0 0 0 |
| −0.038 −0.038 0.496 0 0 0 | −0.033 −0.033 0.422 0 0 0 |
| 0 0 0 0 0.0318 0 0 | 0 0 0 0 0.034 0 0 |
| 0 0 0 0 0 0.0318 0 | 0 0 0 0 0 0.034 0 |
| 0 0 0 0 0 0 0.0318 | 0 0 0 0 0 0 0.034 |

Table 5
Homogenized elastic tensors of auxetic composite No.4.

<table>
<thead>
<tr>
<th>3D Auxetic composite No. 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.3953 −0.112 −0.575 −0.0138 −0.0007 −0.0028</td>
</tr>
<tr>
<td>−0.1112 0.382 −0.0481 0.0215 0.0019 −0.0031</td>
</tr>
<tr>
<td>−0.0575 −0.048 0.4360 −0.005 0.003 0.0124</td>
</tr>
<tr>
<td>−0.0138 0.0215 −0.005 0.0752 0.0018 −0.0026</td>
</tr>
<tr>
<td>−0.0007 0.002 0.0003 0.0018 0.0728 0.001</td>
</tr>
<tr>
<td>−0.0028 −0.003 0.0124 −0.0026 0.001 0.0757</td>
</tr>
</tbody>
</table>

Fig. 26. The optimized topology of 3D auxetic composite microstructure No.4 with two materials.

(a1, a2 and a3) The topologies of M1 and M2 materials, and the final topology, respectively.

(b1, b2 and b3) Cross-sectional views of (a1, a2 and a3), respectively.
6.3.1. Simulation for 2D re-entrant auxetic composite

The optimized 2D re-entrant auxetic composite with two materials, displayed in Fig. 10, is considered in this example. As shown in Fig. 29, the “STL.file” of the 2D auxetic composite microstructure in Fig. 10 is firstly outputted from Matlab software and then imported into ANSYS, which should be converted into the solid geometry with the size of 10 cm × 10 cm × 0.1 cm in the modeling module of ANSYS “SpaceClaim” and then distributed in spatial with a 5 × 5 periodicity. The periodic repetitive composite microstructures briefly work as the auxetic composite in the latter simulation. The finite element mesh of the auxetic composite with the local view is also displayed in Fig. 29(c). Meanwhile, it should be noted that the outputted “STL” files for two materials are separate.
models. After inputting into ANSYS platform, the contact constraints should be imposed on the interfaces between two materials to ensure the latter finite element analysis. In the latter 3D validation, the same manipulation is also performed.

As shown in Fig. 30, four different boundary conditions are imposed on the 2D auxetic composite, namely Conditions 1 to 4. In Condition 1, the X-direction and Z-direction displacements of the left edge are fixed, respectively, namely the displacements equal to 0, shown in Fig. 30(a). Fig. 30(b) fixes the displacements of two points (plotted with the yellow color) located at the middle of the auxetic composite in all directions, which can avoid the rotation of the 2D auxetic composite with the imposing of the load. Condition 3 controls the displacements
of the 2D auxetic composite in Z-direction, equal to 0, which ensure the deformation will be formed in the X-Y plane, shown in Fig. 30(c). Condition 4 is defined in Fig. 30(d), where a displacement 1 mm along $X^+$-direction is homogeneously imposed on the right edge.

As shown in Fig. 31(a) and (b), the displacements of the top and bottom edges are represented, respectively. The average displacements at the top and bottom edges present the deformation degree of the 2D auxetic composite, when a homogeneous displacement is imposed on the edge. The mean value of the displacements on the top edge is equal to 0.302 mm, and the value at the bottom edge is equal to $-0.302$. The deformation of the 2D auxetic composite in Y direction is equal to 0.604 mm. Based on the definition of the Poisson’s ratio, its value can be calculated, equal to $-0.604$. As we can see, the simulated value is mostly identical to the value evaluated by the IGA-based homogenization ($-0.606$). Moreover, the total deformation of the 2D auxetic composite is shown in Fig. 31(c), and the deformed auxetic composite is also displayed in Fig. 31(d), which can show the auxetic behavior of the topologically-optimized 2D auxetic composite. Finally, the dynamic deformation of the 2D re-entrant auxetic composite is attached in Appendix 1.

6.3.2. Simulation for the 3D auxetic composite No.1

In this section, the numerical verification is performed for the 3D auxetic composite No.1 shown in Fig. 20 using ANSYS platform. Based on the optimized result in Section 6.2, the STL files of the auxetic composite microstructure 1 are firstly outputted from the Matlab software, shown in Fig. 32(a) and then imported into the commercial software ANSYS. The STL files for the 3D auxetic composite microstructure 1 should be slightly modified in the modeling software SpaceClaim of ANSYS and converted into the solid geometries with $10 \times 10 \times 10$ cm, shown in Fig. 32(b). The 3D auxetic composite No.1 with the $3 \times 3 \times 3$ repetitive material microstructures will be considered in the
In the simulation, three different boundary conditions are imposed on the 3D auxetic composite No.1. As shown in Fig. 34(a), the displacements of the surface A along Z-direction are fixed, and Condition 2 fixes two points located at the middle of the surface A to avoid the rotation of the auxetic composite No.1, given in Fig. 34(b). The displacement with 1 mm along Z direction is homogeneously imposed on the surface C in Condition 3, shown in Fig. 34(c). It is noted that Surfaces A and C are opposite along Z direction.
As shown in Fig. 35, the displacements at the top and bottom surfaces in X direction are both provided. The difference of the average displacements at the top and bottom surfaces is viewed as the deformation degree of the 3D auxetic composite No.1 in X direction. The average displacement of the bottom surface is equal to $-0.0458$ mm, and the mean value of the displacements at the top surface is equal to $+0.0379$ mm. Hence, the deformation of the auxetic composite No.1 in X direction is $0.0837$. According to the definition of the Poisson’s ratio, the value is equal to $-0.0837$. Hence, the simulated negative Poisson’s ratio is mostly identical to the value evaluated by the IGA-based homogenization. Finally, the dynamic deformation of the 3D auxetic composite No.1 is also attached in Appendix 2.

7. Conclusions

In this paper, an effective and efficient isogeometric topology optimization (ITO) method is proposed for the computational design of auxetic composites with the re-entrant and chiral deformation mechanisms, not only in 2D, but also considering 3D cases. In the ITO method, an IGA-based EBHM is firstly developed, where periodic boundary conditions are imposed on material microstructures. Secondly, a N-MMI model is developed to present the evolving of multi-material topology of microstructures. Finally, a unified ITO formulation for 2D and 3D auxetic composites with different deformation mechanisms is developed, where the objective function with a shift parameter is defined by the homogenized elastic tensor.

Several numerical examples in 2D and 3D are tested to demonstrate the effectiveness and efficiency of the ITO method. A series of novel and interesting auxetic composite microstructures with different deformation features in 2D and 3D are achieved, which can show the superior capability of the ITO method. The effect of weight
parameter in the objective function on the optimization of auxetic composite microstructures has been extensively discussed by the qualitative analysis, which claims the importance of different terms in the objective function. The topologically-optimized auxetic composites in 2D and 3D are also simulated in the ANSYS platform to present the auxetic behavior stemming from the re-entrant and chiral deformation mechanisms. In the future, the proposed ITO method can be extended to discuss other advanced problems, such as micro-architected composites with multi-physical properties, new findings in creating novel properties of artificial materials, and the nonlinear topology optimization for auxetic composites.

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Appendix A. Supplementary data

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References


