

From Spinodal Decomposition to Highly Anisotropic Mechanical Metamaterials: A Novel Design Approach [†]

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Abstract

Mechanical anisotropy plays a crucial role in structural engineering. Conventional periodic lattices offer limited control over anisotropy, largely due to tessellation constraints. Spinodal metamaterials, inspired by the eponymous phase-separation process, provide non-symmetric but periodic and tunable architectures capable of exhibiting strong directional stiffness. In this work, both isotropic and anisotropic spinodal decomposition are modeled, with anisotropy introduced through directional mobility coefficients along the principal spatial axes. The resulting phase fields are converted into STL models and analyzed via finite element-based homogenization to compute directional Young’s moduli. A genetic algorithm identifies parameter combinations that maximize stiffness along a target direction while minimizing it along orthogonal directions. The results demonstrate a direct correspondence between the anisotropy of the spinodal transformation and the mechanical response of the resulting metamaterial, thereby highlighting the advantages of modeling an anisotropic diffusional process, albeit with a greater computational cost.

Keywords: mechanical metamaterials; spinodal topology; Cahn–Hilliard equation; FE mechanical homogenization

1. Introduction

Mechanical anisotropy, namely the directional dependence of material properties, is a desirable feature in many structural applications. Since practical loading scenarios are rarely equiaxial, the ability to tailor stiffness or strength along specific orientations of architected metamaterials represents a clear functional advantage. Traditional periodic lattices have attempted to capture this behavior by tuning geometric parameters [1–3] or by reorienting unit cells [4,5]. Nonetheless, despite considerable progress, the achievable degree of anisotropy continues to be constrained. This limitation arises from the inherent periodicity of these architectures, which restricts tessellation to a finite set of orientations and precludes continuous variation in directional properties [6]. Consequently, periodic lattices often fall short when strong anisotropy is required.

The rapid development of Additive Manufacturing (AM) technologies provides new opportunities to effectively tackle this limitation. AM enables the direct fabrication of extremely complex geometries that were previously unattainable, closing the loop between digital design and physical fabrication [7–10]. This ability has boosted the advent of mechanical metamaterials, defined as artificial materials whose unconventional behavior is



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mostly controlled by their geometry and structure [2,11–14]. Within this rapidly evolving field, non-periodic metamaterials have become increasingly attractive, as they markedly expand the design space compared to traditional lattices. Notably, spinodal-based metamaterials inspired by the phase separation process, mathematically described through the Cahn–Hilliard equation, offer irregular yet continuous topologies that can be systematically controlled. Their non-periodic nature makes them especially promising for generating strong directional properties [6,15,16]. Recent research has demonstrated that spinodal architectures can be tuned to exhibit strong anisotropic responses, thereby overcoming the geometric limitations of periodic structures [16–19].

Motivated by these findings, this work presents a novel computational framework for designing spinodal metamaterials with maximized anisotropy. The proposed workflow integrates three key steps: (i) simulation of spinodal decomposition to generate metamaterial topologies, (ii) finite element-based homogenization to evaluate their mechanical performance, and (iii) multi-objective optimization via a genetic algorithm to identify the parameter set maximizing directional stiffness differences. The goal is to obtain spinodal topologies with improved stiffness along a prescribed direction (x) while reducing it along orthogonal directions (y, z).

The paper is organized as follows: Section 2 introduces the adopted methodology. Section 3 reports and discusses the main results, and Section 4 concludes the work with final remarks and outlook.

2. Methodology

This section outlines the overall workflow of the study. First, the mathematical model that simulates spinodal decomposition, i.e., the physical phenomenon inspiring our metamaterials, is introduced in Section 2.1. Next, the Finite Element (FE) model and the homogenization framework are detailed in Section 2.2. Finally, the optimization strategy developed to design a spinodal metamaterial with the maximum attainable degree of anisotropy is presented in Section 2.3.

2.1. Mathematical Model: Cahn–Hilliard Equation

The process of spinodal decomposition involves the spontaneous separation of a homogeneous mixture into two phases, while preserving the initial 50:50 volume fraction. This process is mathematically described by the Cahn–Hilliard equation [20–25], widely recognized as computationally challenging due to its nonlinearity and stiffness. In this section, a concise overview of the numerical method adopted to solve the equation is provided, while a complete exposition can be found in [26].

Following the approach of [17] with the goal of reducing the number of design parameters, which is critical for the subsequent optimization process, the Cahn–Hilliard equation has been made dimensionless for both isotropic and anisotropic diffusion processes. For brevity, only the dimensionless forms of the equations are presented here.

For the isotropic case, the governing equation becomes:

$$\frac{\partial \phi}{\partial \tilde{t}} = \nabla_{\tilde{x}}^2 \left[-\alpha \beta \nabla_{\tilde{x}}^2 \phi - \beta \phi (1 - \phi^2) \right] \quad (1)$$

where $\phi \in [-1, 1]$ is the phase-field solution; $\tilde{t}$ and $\tilde{x}$ are the dimensionless time and space, respectively; α and β are the dimensionless independent parameters for the isotropic case.

In the anisotropic case, which allows modeling direction-dependent diffusional behavior, the equation reads:

$$\frac{\partial \phi}{\partial t} = \frac{\partial^2}{\partial \tilde{x}^2} \left[-\alpha \beta_x \nabla_{\tilde{x}}^2 \phi - \beta_x \phi (1 - \phi^2) \right] + \frac{\partial^2}{\partial \tilde{y}^2} \left[-\alpha \beta_y \nabla_{\tilde{x}}^2 \phi - \beta_y \phi (1 - \phi^2) \right] + \frac{\partial^2}{\partial \tilde{z}^2} \left[-\alpha \beta_z \nabla_{\tilde{x}}^2 \phi - \beta_z \phi (1 - \phi^2) \right] \quad (2)$$

where the additional dimensionless parameters β_x , β_y and β_z account for the anisotropic diffusion.

The equations described above have been solved using the Finite Difference Method (FDM). Specifically, the time derivative is treated using an explicit forward Euler scheme, while the Laplacian operator is evaluated with a 27-point stencil [27]. The numerical implementation was carried out in MATLAB® R2025b. An example of the resulting phase-field solution, which serves as the starting point for the metamaterial design process discussed in the following section, is shown in Figure 1.

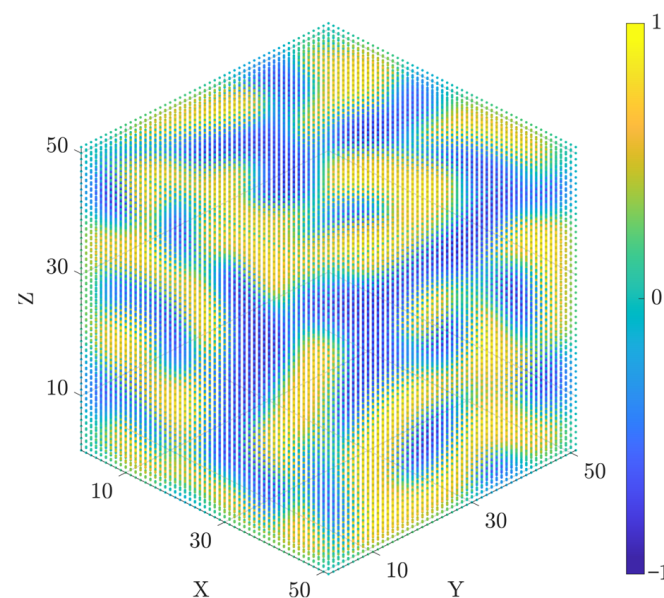


Figure 1. Phase-field solution obtained from Equation (1) with $\alpha = 1.5$ and $\beta = 27.405$.

2.2. Computational Framework: FE Model and Mechanical Homogenization

The FE model of the spinodal metamaterial is constructed directly from the phase-field solution ϕ (similar to that shown in Figure 1), obtained by solving the Cahn–Hilliard equation in either isotropic (Equation (1)) or anisotropic form (Equation (2)). In our work, the material domain is defined where ϕ is negative.

In order to transform the raw phase-field solution into a robust computational mesh, an automated workflow has been implemented in MATLAB®: first, an iso-surface is extracted and exported as an STL geometry, which is then subjected to a cleaning and correction process to eliminate potential topological inconsistencies and enhance tessellation uniformity.

The corrected surface is subsequently discretized into a volume mesh using high-order tetrahedral elements via Gmsh 4.14 [28], allowing direct meshing from the triangulated surface without requiring an underlying CAD model. The resulting mesh is finally exported in a solver-compatible format for FE simulations (CDB format in this work). Figure 2 provides an example of the obtained STL model (a) and the FE mesh (b).

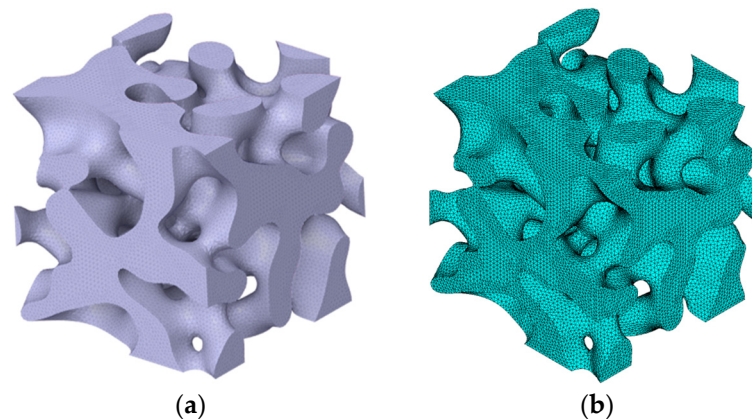


Figure 2. Example of the metamaterial model obtained from Equation (1) with $\alpha = 1.5$ and $\beta = 27.405$: (a) STL model; (b) FE mesh.

The mechanical characterization of the metamaterial is carried out via computational homogenization, a well-established technique to determine the behavior of non-homogeneous materials. The key step in this method is the definition of a Representative Volume Element (RVE), from which averaged stress and strain fields are extracted and subsequently used to compute effective elastic constants [29–32]. Among the boundary conditions that can be applied, periodic boundary conditions (PBCs) are generally regarded as the most reliable, as they provide a realistic representation of the material response [30,31,33–35]. However, their implementation requires establishing node-to-node correspondence on the opposite faces of the RVE and introducing constraint equations to couple the displacements of these nodes in order to simulate the behavior of a unit cell embedded in an infinite domain. This predictably results in a significant increase in the computational cost of the homogenization procedure. In contrast, displacement boundary conditions (DBC) are simpler to implement and widely used in homogenization procedures, particularly when the objective is to determine Young's moduli. This has been extensively documented in the literature [36,37], and we have previously shown that, even in the case of spinodal metamaterials, DBCs yield Young's modulus values equivalent to those obtained with PBCs [26]. For this reason, DBCs have been adopted throughout the present study.

2.3. Unconstrained Optimization of Mechanical Anisotropy

The modeling and FE-homogenization framework described above was integrated into an optimization workflow, including 250 iterations, aimed at identifying spinodal metamaterial configurations that maximize mechanical anisotropy. The optimization is unconstrained, focusing solely on enhancing the contrast between the stiffnesses along the principal directions, both for metamaterials derived from isotropic and anisotropic spinodal processes.

Due to the complexity of the design space, a gradient-free (Heuristic) optimization strategy was employed. Therefore, a Genetic Algorithm (GA) was chosen for its ability to explore design spaces without relying on gradient information and to converge toward near-optimal solutions through stochastic operations.

The design variables are α and β in the isotropic case (from Equation (1)), and α together with the direction-dependent parameters β_x , β_y , and β_z in the anisotropic case (from Equation (2)). These parameters directly control the morphology of the spinodal metamaterial, and thus its mechanical behavior. Their admissible ranges are adopted from our previous study [26].

For each candidate solution, the Young's moduli E_{xx} , E_{yy} , and E_{zz} are extracted. The optimization objective is expressed as the maximization of two anisotropy indices: the ratios of the Young's modulus along the x direction to those along the y and z directions (E_{xx}/E_{yy} and E_{xx}/E_{zz} , respectively). The GA seeks to maximize these indices without imposing additional constraints on the absolute values of the moduli. This unconstrained optimization is intended to demonstrate the ability of spinodal metamaterials to generate directional stiffness, providing a clear framework for analyzing how isotropic and anisotropic diffusional processes influence mechanical performance. The results of the optimization process are presented in the next section.

3. Results and Discussion

In this section, the results are presented and discussed to assess whether introducing anisotropy into the underlying diffusional process of spinodal metamaterials effectively promotes mechanical anisotropy in the resulting material properties.

Figure 3 shows the distribution of mechanical anisotropy ratios (i.e., E_{xx}/E_{yy} and E_{xx}/E_{zz}) for metamaterials derived from both isotropic and anisotropic spinodal processes. In the isotropic case, the ratios E_{xx}/E_{yy} and E_{xx}/E_{zz} are always limited to values below 1.5, reflecting a nearly uniform mechanical response along the three principal directions. In sharp contrast, in the anisotropic case these ratios can reach values of up to 5, indicating a significant mechanical anisotropy. These trends are numerically summarized in Table 1, which reports the maximum values of anisotropy ratios obtained for both cases.

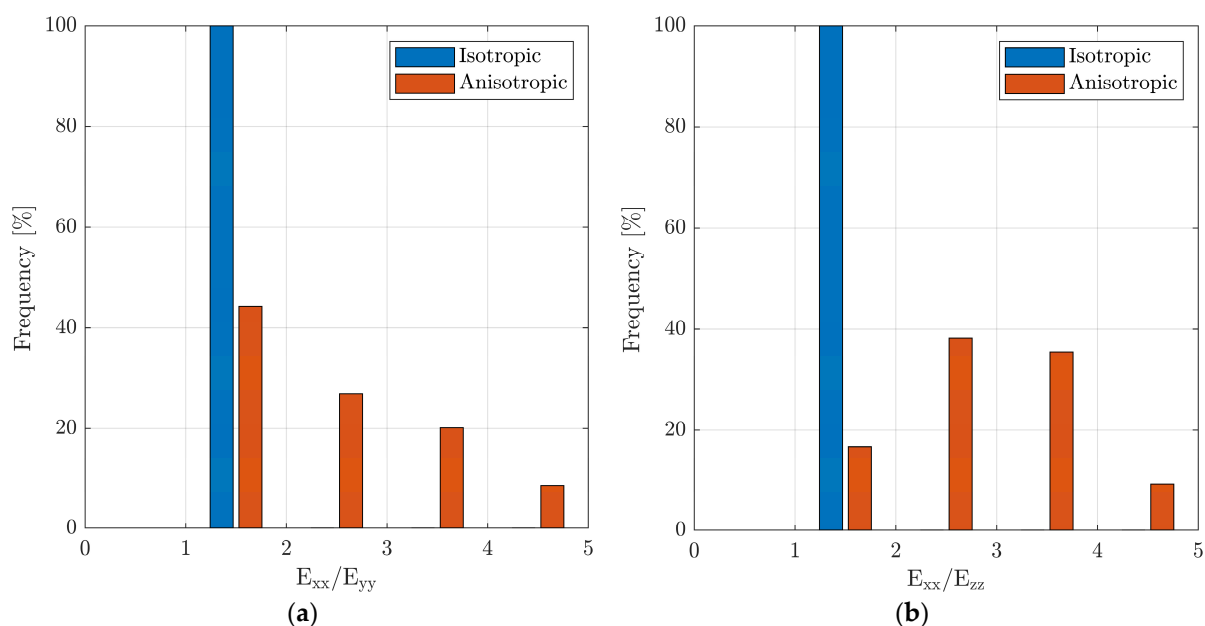


Figure 3. Distribution of mechanical anisotropy ratios for metamaterials derived from isotropic (blue) and anisotropic (orange) spinodal process: (a) E_{xx}/E_{yy} ; (b) E_{xx}/E_{zz} .

Table 1. Maximum anisotropy ratios for metamaterials derived from isotropic and anisotropic spinodal processes.

Mathematical Model	Max E_{xx}/E_{yy}	Max E_{xx}/E_{zz}
Isotropic—Equation (1)	1.420	1.482
Anisotropic—Equation (2)	4.975	4.895

Figures 4 and 5 show spider plots of the Young's moduli for the isotropic and anisotropic cases, respectively. This representation provides an immediate visual un-

derstanding of the directional mechanical response of the selected metamaterials. Figure 4 shows the metamaterial derived from Equation (1) with maximum E_{xx}/E_{yy} , displaying nearly identical values along the y and z directions: E_{xx} is only approximately 45% higher than E_{yy} and E_{zz} . This is consistent with the limited anisotropy observed in this case (Figure 3a).

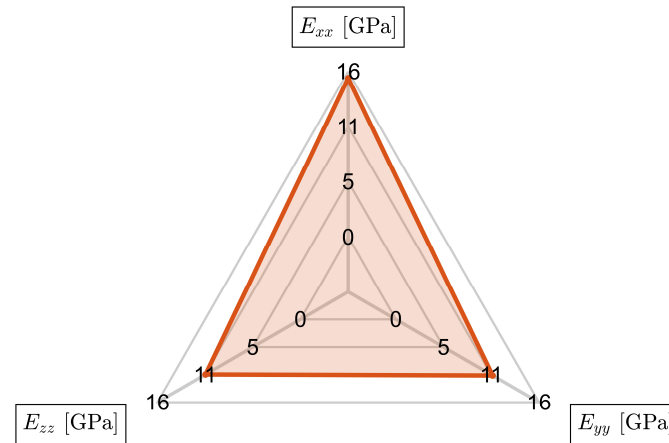


Figure 4. Spider plot of Young's moduli for the metamaterial with maximum E_{xx}/E_{yy} derived from isotropic spinodal process.

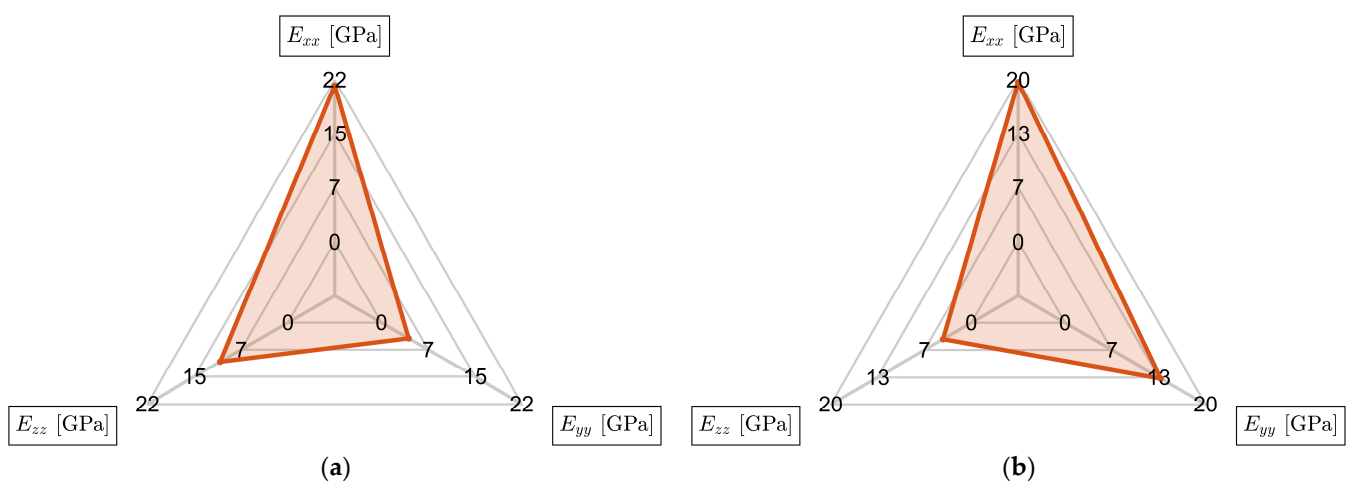


Figure 5. Spider plot of Young's moduli for the metamaterial derived from anisotropic spinodal process: (a) with maximum E_{xx}/E_{yy} ; (b) with maximum E_{xx}/E_{zz} .

Figure 5 shows the metamaterial derived from Equation (2) with maximum E_{xx}/E_{yy} (Figure 5a) and E_{xx}/E_{zz} (Figure 5b), highlighting a pronounced directional mechanical behavior: E_{xx} is approximately 300% higher than E_{yy} and E_{zz} .

To better understand how mechanical anisotropy is affected by the design parameters, Figure 6 shows the correlation matrix between the design parameters and the anisotropic ratios for metamaterials derived from Equation (2). This representation provides insight into the influence of α , β_x , β_y , and β_z on the mechanical properties and guides parameter tuning to achieve desired stiffness distributions. The matrix reveals that β_z exhibits the strongest correlations with the directional moduli: positively with E_{xx} (0.79) and E_{zz} (0.86), and negatively with E_{yy} (−0.95), confirming its critical role in controlling the stiffness contrast along the three axes. Similarly, β_x shows a moderate positive correlation with E_{xx} (0.65), suggesting that increasing β_x enhances stiffness along the x direction. In contrast, β_y has weaker correlations with the directional moduli, indicating a more limited influence

on the overall mechanical anisotropy. The global parameter α shows only moderate correlations with E_{xx} (0.50) and smaller correlations with E_{yy} (−0.34) and E_{zz} (−0.04).

α	1.00	0.65	−0.27	0.31	0.50	−0.34	−0.04
β_x	0.65	1.00	−0.20	0.25	0.65	−0.08	−0.20
β_y	−0.27	−0.20	1.00	0.00	−0.38	0.08	0.23
β_z	0.31	0.25	0.00	1.00	0.79	−0.95	0.86
E_{xx}	0.50	0.65	−0.38	0.79	1.00	−0.68	0.45
E_{yy}	−0.34	−0.08	0.08	−0.95	−0.68	1.00	−0.87
E_{zz}	−0.04	−0.20	0.23	0.86	0.45	−0.87	1.00
	α	β_x	β_y	β_z	E_{xx}	E_{yy}	E_{zz}

Figure 6. Correlation matrix between design parameters (α , β_x , β_y , and β_z) and Young's moduli (E_{xx} , E_{yy} and E_{zz}) for metamaterials derived from anisotropic spinodal process.

Overall, these results quantitatively demonstrate that isotropic spinodal processes produce nearly uniform material stiffness, whereas anisotropic processes allow the design of metamaterials with highly directional mechanical properties. In addition, these correlations confirm that the anisotropic mobility parameters directly govern the directional mechanical properties: proper adjustment of β_x , β_y and β_z allows fine-tuning of the stiffness along each principal direction.

4. Conclusions

This work investigates whether modeling an anisotropic spinodal decomposition process can produce metamaterials with a pronounced anisotropic mechanical response. To this end, a computational framework was developed, consisting of three main steps:

1. Solution of the non-linear Cahn–Hilliard PDE using a finite difference numerical algorithm, yielding a phase-field solution that serves as the starting point for the spinodal-inspired metamaterial design process.
2. FE modeling and homogenization to calculate the Young's moduli of the resulting metamaterial.
3. Unconstrained optimization based on a genetic algorithm, aimed at maximizing anisotropy ratios (E_{xx}/E_{yy} and E_{xx}/E_{zz}).

The results demonstrate that isotropic spinodal processes yield a quasi-isotropic mechanical response, with only residual anisotropy along the principal directions. In contrast, introducing anisotropy into the underlying diffusion process significantly enhances directional mechanical response, with stiffness ratios (E_{xx}/E_{yy} and E_{xx}/E_{zz}) up to five times greater than those in the isotropic case. Correlation analysis further reveals that the directional mobility parameters (β_x , β_y , β_z) play a pivotal role in governing the mechanical response along each axis. In particular, β_z was identified as the most influential parameter, strongly controlling stiffness contrast among the three directions, while β_x and β_y provide additional tuning capabilities. These findings offer preliminary design guidelines for spinodal-inspired metamaterials with tailored anisotropic response.

Overall, this work shows that incorporating anisotropy into spinodal decomposition provides a powerful strategy for creating metamaterials with enhanced directional stiffness and tunable mechanical properties.

As future developments, the proposed design approach could be extended to multifunctional spinodal-inspired metamaterials, for instance, by simultaneously targeting anisotropic thermal conductivity alongside mechanical anisotropy. The ability to tune diffusional parameters to achieve specific mechanical and thermal behaviors could unlock new opportunities in both structural and energy-related applications. Furthermore, incorporating more sophisticated optimization objectives, including multi-physics constraints, would further broaden the versatility of spinodal-inspired metamaterial design.

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