A continuum model for nonlinear lattices under large deformations

Raj Kumar Pal\textsuperscript{a}, Massimo Ruzzene\textsuperscript{a,b}, Julian J. Rimoli\textsuperscript{a,*}

\textsuperscript{a}School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States
\textsuperscript{b}School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

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\section*{ABSTRACT}

A continuum model is developed for hexagonal lattices, composed of a set of masses connected by linear axial and angular springs, with nonlinearity arising solely from geometric effects. For a set of lattice parameters, these lattices exhibit complex deformation patterns under uniform loading conditions due to instabilities. A continuum model accounting for these instabilities is developed from explicit expressions of the potential energy functional of a unit cell. This functional is non-convex, it captures the bistable nature of the lattice, and is used to derive its effective constitutive behavior. Finite element simulations of continuum medium illustrate the formation of microstructural patterns with discontinuous displacement gradients, similar to the features observed in nonlinear elasticity and finite deformation plasticity. A comparison of discrete lattice simulations and finite element analysis under general loading conditions illustrates that the continuum model captures the effective behavior due to instabilities within the lattice.

\section*{1. Introduction}

The physics of lattice-based material models has been an active area of research for the past few decades. These models are used to study a wide range of physical phenomena, from atomic models of materials \textcitep{Keating1966} to truss structures \textcitep{Wadley2003} to granular media \textcitep{Cundall1979}. In recent years, focus has been placed on designing tailored lattices for attaining specific objectives \textcitep{Evans2001} such as lightweight, heat dissipation and multifunctionality. There have primarily been two approaches for modeling lattices. The first approach, pioneered by \textcitep{Gibson1982,Gibson1997}, models lattice materials as slender beams and has been applied extensively to study two-dimensional (2D) hexagonal, square and chiral lattice topologies. The second approach considers lumped parameter models consisting of spring networks and point masses. In this category, the Kirkwood-Keating model \textcitep{Kirkwood1939} has been extensively used, for example, to study properties of polymer molecules \textcitep{Tasumi1962}, atomic lattices \textcitep{Rucker1995}, and percolation in elastic media \textcitep{Kantor1984}.

Buckling and instabilities arising in lattices undergoing large deformations have been extensively studied. \textcitep{Ohno2002} derived conditions for the onset of microscopic bifurcation in finite deformation lattices based on the principle of virtual work. The authors illustrated numerically that the superposition of buckling modes can result in complex patterns. \textcitep{Triantafyllidis1993, Triantafyllidis1996, Triantafyllidis1999, Triantafyllidis2001} developed a two-scale homogenization procedure to study microscopic buckling and post-buckling behavior of periodic elastoplastic cellular solids, \textcitep{Tadmor1999} developed homogenization of three-dimensional (3D) atomic lattices with convex potentials to derive bulk properties and behavior of materials. \textcitep{Arroyo2002} extended this method to model thin sheets of atoms undergoing bending and stretching and applied it to study graphene sheets and carbon nanotubes. Although the potentials used in molecular dynamics simulations are convex, loss of ellipticity leading to material instability, can arise due to large deformation geometric nonlinearity. Later, \textcitep{Arroyo2008} incorporated an equivalent beam model with non-convex strain energy functional into their framework to model the wrinkling phenomena observed experimentally in thick carbon nanotubes. \textcitep{Miehe2002} developed a homogenization procedure for periodic composites undergoing large deformations and exhibiting both structural (buckling) and material (due to non-convexity) instabilities.
Non-convex strain energy functionals arise in nonlinear elastic media (Ball and James, 1987) and their study has supported the investigation of phase transitions in shape memory alloys (Bhattacharya, 1993; 2003) and in finite deformation plasticity, where microstructure forms patterns minimizing the overall energy of the structure. Examples include internally twinned martensite (Ball and James, 1987), shear and slip bands (Aifantis, 1987), laminate micro-structures (Dmitrieva et al., 2009), and Lüders bands (Mesarovic, 1995). These patterns feature layers of homogeneously deformed regions which can range from atomistic (slip in crystalline materials) to macroscopic (kink bands in sheets of paper (Hunt et al., 2000)), to geological scales (chevron folds in rocks (Conti and Hackl, 2015)), and play a key role in the mechanical behavior of the medium by influencing material properties across the length scales.

In the discrete domain, non-convex potentials also occur in the case of bistable lattices, which have been subject of recent interest due to their suitability for the development of diverse engineering applications, including tunable metamaterials (Schaaffler and Ruzzene, 2015), smart morphing structures (Schultz, 2007), and deployable shells and structures (Schioler and Pellegrino, 2007). Although some research has been conducted on the mechanics of one-dimensional (1D) bistable lattices, e.g., (Cherkaev et al., 2005; Restrepo et al., 2015), limited attention has been devoted to models and guidelines for higher dimensional bistable lattices. An interesting example in this category is the 2D hexagonal lattice, which is topologically equivalent to the re-entrant configuration. Though the stability and linearized small deformation behavior of both these lattices have been investigated extensively (Ostoja-Starzewski, 2002), there is a paucity of works in the literature demonstrating the mechanics of transition from one configuration to the other.

In the present work, we develop a constitutive model for lattices capable of transforming from the hexagonal to the re-entrant configuration, and adopt it to demonstrate parallels between instabilities in discrete lattices and microstructural patterns in continuum media governed by non-convex potentials. The lattice is modeled as a network of linear axial and angular springs, undergoing large deformations. We illustrate how non-convex potential energy functionals and complex phenomena like snap-through instability can arise solely as a consequence of geometric nonlinearity. Moreover, these functionals lead to complex patterns in finite discrete lattices and microstructure features in the corresponding homogenized continuum medium. We demonstrate the applicability of the homogenization approach to study large lattice structures using finite element methods.

The outline of the paper is as follows: In Section 2, the lattice is described along with numerical simulations illustrating key phenomena. Next, an analytical solution for the potential energy functional of a lattice unit cell is derived. In Section 3, homogenized constitutive law for an equivalent hyper-elastic material are derived using this potential energy functional. Section 4 presents the behavior of large finite lattices and compares with the response of equivalent continuum media. Multiple examples are presented demonstrating the ability of the homogenization procedure to predict the behavior of the lattice under complex loading conditions. Finally, the key findings of this work are summarized in Section 5, which also outlines directions of future research.

2. Discrete lattice under finite deformation

We consider lattices that are hexagonal in their un-deformed configuration. The lattices have the ability to deform and transition to the topologically equivalent re-entrant configuration. Fig. 1(a) and (b) illustrate, respectively, the schematic of a hexagonal and a re-entrant cell configuration. Note that our un-deformed lattice only exhibits 4-fold rectangular symmetry as opposed to the 6-fold symmetry associated with a regular hexagonal lattice. The configuration is called hexagonal when all the interior angles are greater than π/2 and is termed re-entrant when at least one interior angle is less than π/2. For a certain set of lattice parameters and a range of strain values, we demonstrate that complex patterns form in the interior of a finite sized lattice even when subjected to affine deformation at the boundary. The description of these patterns form the motivation for developing a continuum model and this model is intended to capture the effective behavior of the lattice when these patterns arise. In this section, we first introduce the lattice and its non-dimensional parameters. We then illustrate through numerical simulations typical behaviors associated with these lattices, which serve to motivate the development of our continuum model.

2.1. Lattice configuration

The system under study is a planar 2D hexagonal lattice network, composed of a collection of M nodes, connected by N edges. Each interior node is connected by 3 edges to adjacent nodes and each boundary node is connected by 2 edges, which ensures that there are no hanging nodes in the lattice. The nodes have point masses, while the edges are massless linear springs that resist the change in length of the edge. In addition, angular springs at the nodes resist relative angular motion of every two adjacent edges connected at the node. All the axial springs have identical undeformed lengths L. Both the axial and angular springs are undeformed in the hexagonal lattice configuration. We assume that all the springs have identical angular and axial stiffness, denoted k_x and k_l, respectively. The degrees of freedom of the lattice are the nodal coordinates \( \mathbf{x}_i = (x_{i}, y_{i}) \), \( i = 1, 2, \ldots, M \).

Consider two edges p and q spanned by nodes (i, j) and (i, k), respectively, with a common node i shown in Fig. 1. The angle \( \beta_{pq}^i \) between the edges is related to the degrees of freedom by the kinematic relation:

\[
\cos(\beta_{pq}^i) = \frac{(\mathbf{x}_j - \mathbf{x}_i, \mathbf{x}_k - \mathbf{x}_i)}{|\mathbf{x}_j - \mathbf{x}_i| |\mathbf{x}_k - \mathbf{x}_i|},
\]

where \((\cdot, \cdot)\) and \(|\cdot|\) denote, respectively, the scalar product and l2 norm of the vectors. Let \( \Delta \beta_{pq}^i \) denote the change in this angle between edges (p, q) and let \( \Delta L_{pq}^i \) be the change in length of an axial spring on edge m connecting nodes i and j, expressed as:

\[
\Delta L_{pq}^i = |\mathbf{x}_j - \mathbf{x}_i| - L.
\]

The potential energy of the lattice is given by

\[
E = E_a + E_l = \sum_{m=1}^{N} \frac{1}{2} k_{a}(\Delta L_{pq}^m)^2 + \sum_{i=1}^{M} \sum_{p=q}^{M} \frac{1}{2} k_{l}(\Delta \beta_{pq}^i)^2,
\]

where the first term is the energy associated with the axial springs, with the index m summing over all the edges of the lattice and (i, j) are the nodes spanning edge m. The second term is the energy from the angular springs, with index i summing over the nodes and index e summing over all adjacent pairs of edges (p, q) at node i. It is observed that the energy is frame invariant and does not change under rigid translations and rotations. Thus, it can be used to study large displacement effects.

For a prescribed set of boundary conditions, a stable equilibrium configuration is obtained by minimizing the energy E with respect to the degrees of freedom, i.e., the position of the unconstrained nodes. Since the problem is nonlinear, there is a possibility of multiple stable and unstable equilibrium configurations. The specific configuration attained depends on the particular loading path imposed on the lattice. We express all physical quantities in non-dimensional form by normalizing the position vectors \( \mathbf{x} \) by L,
which is a characteristic length scale of the lattice, and introducing a non-dimensional angular stiffness \( \eta \) based on the ratio of the angular stiffness to the axial stiffness:

\[
\mathbf{x} \rightarrow \frac{\mathbf{x}}{L}, \quad \eta = \frac{k_t}{k_L a^2}.
\]

The energy and thus the static properties of the system are expressed in terms of this material parameter \( \eta \) and the initial geometric configuration of the lattice.

### 2.2. Numerical solutions illustrating finite deformation patterns

#### 2.2.1. Approach

We illustrate some of the complex behaviors that typically arise in a finite-sized hexagonal lattice, whose description by a continuum model is the focus of our study. This illustration is done by numerical simulations on a discrete lattice, composed of 168 nodes and 67 cells. Accompanying these simulations of the lattice, we also present numerical simulations on a unit cell, which provide insight into the physics of the solution. Fig. 1(d) displays a unit cell of the lattice in the un-deformed configuration. In all of our numerical simulations, the angle \( \psi \) between the edges 1 and 2 in the unit cell oriented as shown in Fig. 1(d), is chosen to be \( 5\pi/6 \) in the un-deformed configuration. Note that this angle is \( 2\pi/3 \) for a regular hexagonal lattice, while a different value is chosen in the present work so that the masses do not touch when the lattice attains a re-entrant configuration. However, the general trends presented here are applicable to a lattice with any angle that can transform from the hexagonal to re-entrant configurations.

For quasistatic boundary value problems, the equilibrium equation for node \( i \), having an external force \( F_e \) acting on it is \( F_e = \partial E/\partial x_i \). Explicit expressions for the derivative of energy with respect to the nodal coordinates \( x \) can be evaluated using Eqs. (1)–(3). The boundary value problem is nonlinear and is solved by imposing the prescribed displacement or force at the boundary nodes in incremental steps. At each step, a Newton Raphson procedure is used to obtain an equilibrium solution. The eigenvalues of the stiffness matrix (Hessian of the energy functional evaluated at this equilibrium configuration) are computed and the stiffness matrix is checked for positive definiteness to ensure that the solution is a stable equilibrium configuration. If the lowest eigenvalue is negative, then the step size is reduced and a new equilibrium is solved for. If the lowest eigenvalue is zero, then the nodes of the lattice are perturbed by the eigenvector corresponding to this zero eigenvalue and a new equilibrium solution is determined. This perturbation by the eigenvector is motivated by the physical behavior of the lattice at the onset of bifurcation, as the eigenvector is a zero energy displacement mode and the lattice deforms in this direction. As the lattice deforms, the stiffness matrix is modified and a new equilibrium is established. If the Newton-Raphson iterations fail to converge, then a method of steepest descent is used along with an Armijo line search to evaluate the solution. The above method ensures that a local energy minimum is found at every solution step close to the previous solution step. Finally, we note that since the problem is nonlinear, there is a possibility of multiple minimum energy configurations. As the displacement is prescribed in small steps, the final configuration depends on the loading path as the lattice deforms quasistatically from the un-deformed configuration. Note that the solver does not seek a global energy minimum, but seeks a local minimum at each step.

We solve the problem of uniaxial compressive strain \( \beta \) imposed on the \( y \)-direction of the lattice for 3 distinct non-dimensional angular stiffness values \( \eta \). The lattice configuration is solved as a displacement prescribed quasistatic problem, with both components of displacement prescribed on all the boundary nodes, corresponding to an affine deformation field derived from the strain \( \beta \). Note that though an affine deformation field is prescribed on the boundary nodes, the interior nodes may have energy minimizing non-uniform displacement field beyond a bifurcation point. The corresponding numerical solution on the unit cell RVE is done by prescribing the displacement at the nodes 1, 2, 3.

#### 2.2.2. Results

Figs. 2 (a)–(i) display the lattice in the deformed configuration along with an outline (red/light rectangle) of the un-deformed configuration for different strain and non-dimensional angular stiffness values, showing distinct patterns in the displacement field. Fig. 2(a) also illustrates the un-deformed configuration in the background. We will discuss these results in the context of the convexity of the potential energy functional in a unit cell and illustrate that non-affine patterns arise when the energy functional does not coincide with its rank-one convex envelope at the considered strain state. This condition corresponds to the loss of strong ellipticity of the Hessian of the energy \( (\partial^2 E/\partial \mathbf{F} \partial \mathbf{F}) \), where \( \mathbf{F} \) is the local deformation gradient. Indeed, the bifurcations observed in our study are all caused by long wavelength instability modes, where the loss of microscopic stability is associated with the violation of strong ellipticity condition of the homogenized modulii (Geymonat et al., 1993). Fig. 3 illustrates the variation in potential energy of a unit cell with compressive strain \( \beta \) for 3 distinct values of non-dimensional angular stiffness. For low values of \( \eta \) (\( \eta = 0 \)), the potential energy is non-monotone, with the system having an unstable equilibrium and two stable equilibrium positions. Note that the derivative \( \partial E/\partial \beta = 0 \) at each equilibrium position. The stable positions correspond to the hexagonal and the re-entrant geometries and the unstable equilibrium explains the snap-through instability obtained during transition in the lattice. The snap-through instability (Pecknold et al., 1985; Rajasani et al., 2015) describes the dynamic behavior observed in a lattice as it jumps from an unstable to a stable equilibrium configuration. As \( \eta \) increases, the response becomes monotone (e.g. \( \eta = 2 \times 10^{-3} \)), however, the potential energy variation with strain is not convex.
Fig. 2. Deformed configuration of the lattice under uniaxial strain for 3 different \( \eta \) values, showing complex pattern formation in the transition to re-entrant configuration.

![Deformed configuration of the lattice under uniaxial strain for different \( \eta \) values](image)

Fig. 3. Potential energy of unit cell with compressive strain for three angular stiffness values. The points corresponding to the various strain states considered in Fig. 2 are marked on the potential energy plots.

![Potential energy of unit cell with compressive strain](image)

along the loading direction, i.e., not rank-one convex. As the value of \( \eta \) increases further, for example \( \eta = 2 \times 10^{-2} \) in Fig. 3, the potential energy of the unit cell again coincides with its rank-one convex envelope for the considered strain values under uniaxial compression.

We now turn attention to the analysis of deformation in the finite lattice for the 3 non-zero values of \( \eta \) studied above. For low values of strain close to the hexagonal configuration, the displacement of interior nodes is uniform throughout the domain for all values of \( \eta \). However, with increasing strain, the displacement solution is distinct in the 3 cases, as observed for the strain values \( \beta = 0.2 \) in Fig. 2. Fig. 2(a)–(c) display the deformed shapes for a lattice with non-dimensional angular stiffness \( \eta = 2 \times 10^{-2} \) at three distinct strain levels. The displacement field is observed to be uniform in the interior for all strain values as the lattice transforms from hexagonal to re-entrant configuration. Fig. 2(d)–(f) illustrate the deformed configuration of a lattice with non-dimensional angular stiffness \( \eta = 8 \times 10^{-3} \) at the same strain levels. For low values of strain, the displacement field is uniform. As the strain increases, the displacement of the interior nodes is not uniform and patterns arise in the lattice. These local patterns arise as a result of instabilities due to long wavelength bifurcation modes (similar to Triantafyllidis and Bardenhagen (1996); Triantafyllidis and Schnaidt (1993)) and they are influenced by the boundary condi-
tions and the dimensions of the whole lattice. Indeed, the formation of instabilities is associated with the loss of strong ellipticity of the Hessian of the potential energy functional, which is demonstrated above for the unit cell as the potential energy deviates from its rank-one convex envelope and these patterns result in minimizing the total energy of the structure.

As the strain increases further, the lattice attains a re-entrant configuration and the displacement within the lattice again becomes uniform, as illustrated in Fig. 2(f) for \( \beta = 0.4 \). At this high strain value, the potential energy matches again with its rank-one convex envelope and the corresponding Hessian is strongly elliptic. Fig. 2(g) illustrates the deformed shape at a low strain \( \beta = 0.1 \) for the lattice with \( \eta = 2 \times 10^{-3} \). Patterns distinct from the earlier case are observed here for this low value of strain. The patterns grow in amplitude, as observed in Fig. 2(h), before disappearing as the Hessian of the potential energy satisfies strong ellipticity again and the lattice attains the re-entrant configuration. Fig. 2(i) illustrates the deformed lattice shape at the strain level \( \beta = 0.4 \), showing that the patterns become smaller in amplitude as the lattice transitions to re-entrant configuration.

As observed in the unit cell analysis above, the formation of non-affine patterns in a finite lattice is associated with the loss of microscopic stability arising due to the non-quasiconvexity of the potential energy functional. In the present work, all the lattice instabilities which result in complex patterns correspond to the long wavelength bifurcation mode. Thus the lattice deformation is uniform under an affine boundary condition as long as the Hessian of the energy functional satisfies strong ellipticity.

### 3. Continuum model

We demonstrated numerically the transition from hexagonal to re-entrant configuration in the lattice. An interesting feature is the formation of global patterns for low values of the non-dimensional angular stiffness \( \eta \) in contrast to a uniform deformation field for higher \( \eta \). Furthermore, a uniform deformation field is recovered in the re-entrant configuration. In this section, we develop a continuum model, which can capture all of these features and predict the lattice behavior under complex loading conditions.

We start by developing an analytical expression for the strain energy density functional of the equivalent continuum medium. The corresponding stress, tangent stiffness tensors, and variational formulation for the continuum medium are then derived. The energy functional is then verified using the numerical solution of a unit cell of the discrete lattice, and finally, some of the salient features of this functional are discussed.

#### 3.1. Potential energy functional

We derive analytical expressions for the potential energy in the unit cell of the lattice under an imposed deformation gradient \( \mathbf{F} \). This involves solving for the equilibrium configuration of the unit cell. Consider the unit cell shown in Fig. 1(d) with the lattice vectors denoted by \( \mathbf{a}_1, \mathbf{a}_2 \) and the origin of the local coordinate system fixed at node \( \mathbf{x}_j \). From the polar decomposition theorem \((\text{Gurtin, 1982})\), any deformation gradient \( \mathbf{F} \) can be uniquely decomposed into a symmetric and positive definite stretch part \( \mathbf{U} \) and a proper orthogonal rotation part \( \mathbf{R} \) as \( \mathbf{F} = \mathbf{RU} \). Since the energy is zero under rigid rotations in our model, it suffices to provide the strain energy under symmetric deformation \( \mathbf{U} \). Let the normal and shear components of strain be characterized by parameters \((\alpha, \beta, \gamma)\), such that the stretch part of the deformation gradient is given by

\[
\mathbf{U} = \begin{bmatrix} 1 + \alpha & \gamma \\ \gamma & 1 + \beta \end{bmatrix}.
\]  

The corresponding deformation field is imposed on the boundary nodes \((\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)\) of the unit cell and they are held fixed, while the interior node is free to move to satisfy the equilibrium condition. In the deformed configuration, the coordinates of the boundary nodes are

\[
\mathbf{x}_1 = \mathbf{Ua}_1, \quad \mathbf{x}_2 = \mathbf{Ua}_2, \quad \mathbf{x}_3 = \mathbf{0}.
\]  

We first solve for the equilibrium position \( \mathbf{x} = (x, y) \) of the interior node, which will be then utilized to compute the potential energy of the unit cell. Let the set of angular springs between edges be denoted by \( s = \{12, 23, 31\} \) and let \( \theta_{pq}^0 \) denote the angle between the edges \( p \) and \( q \) in the un-deformed equilibrium configuration. For a prescribed deformation gradient \( \mathbf{U} \), the change in length of edges and the angles between them are functions of \((x, y)\) and we denote them by

\[
\Delta d_p(x, y) = \sqrt{(x - x_p)^2 + (y - y_p)^2} - L_p,
\]  

\[
\Delta \theta_{pq}(x, y) = \cos^{-1} \left( \frac{(x - x_p)(x - x_q) + (y - y_p)(y - y_q)}{L_pL_q} \right) - \theta_{pq}^0.
\]  

where, \( L_p = \Delta d_p(x, y) + L \). Finally, the variables \( s_p = \Delta d_p(0, 0) + L \) and \( \theta_{pq}^0 = \theta_{pq}(x, y) \) are introduced for brevity of the expressions.

The potential energy in the unit cell \( E \) in non-dimensional form is given by

\[
E = \frac{1}{2} \sum_{i=1}^{3} (l_i - L)^2 + \eta \sum_{p\in S} \Delta \theta_{pq}^2.
\]  

Note that the angular energy is multiplied by a factor 2 to account for the angular springs at the boundary nodes of the unit cell, which are shared with its neighbors, assuming that the deformation is identical in the neighboring unit cells. To further elucidate on this extra factor, consider an equivalent unit cell obtained by translating the current unit cell along \( y \)-axis by \( -L \). This equivalent unit cell has no boundary nodes and thus avoids the difficulty of counting angular springs which are shared with adjacent unit cells. It has two interior nodes and thus 6 angular springs. Note that the energy due to three angular springs at a node will be the same across all neighboring nodes, as they have identical deformation. Thus, there is a factor 2 for the energy due to angular springs at the interior node in Eq. (8). The equilibrium conditions are given by the stationary points of energy with respect to the coordinates of \( \mathbf{x} \), leading to

\[
\frac{\partial E}{\partial x} = \frac{3}{2} \sum_{i=1}^{3} (l_i - L) \frac{\partial l_i}{\partial x} + \eta \sum_{p\in S} \Delta \theta_{pq} \frac{\partial \theta_{pq}}{\partial x} = 0,
\]  

\[
\frac{\partial E}{\partial y} = \frac{3}{2} \sum_{i=1}^{3} (l_i - L) \frac{\partial l_i}{\partial y} + \eta \sum_{p\in S} \Delta \theta_{pq} \frac{\partial \theta_{pq}}{\partial y} = 0.
\]  

The derivatives with respect to the interior nodal coordinates \((x, y)\) are given by

\[
\frac{\partial l_i}{\partial x} = \frac{x - x_i}{l_i}, \quad \frac{\partial l_i}{\partial y} = \frac{y - y_i}{l_i}.
\]  

\[
\frac{\partial \theta_{pq}}{\partial x} = \frac{\partial \theta_{pq}}{\partial x_p} \frac{\partial x_p}{\partial x}, \quad \frac{\partial \theta_{pq}}{\partial y} = \frac{\partial \theta_{pq}}{\partial y_p} \frac{\partial y_p}{\partial y}.
\]  

The derivatives of angles \( \theta_{pq} \) are expressed in terms of the derivatives with respect to the boundary nodes. These expressions are easily obtained from geometry, for instance, by considering infinitesimal displacements of the nodal coordinates in Fig. 1(c) and are given by:
\[ \frac{\partial \theta_{pq}}{\partial x_p} = -\frac{y_p - y}{l_p^2}, \quad \frac{\partial \theta_{pq}}{\partial y_p} = \frac{x - x_p}{l_p^2}, \]
\[ \frac{\partial \theta_{pq}}{\partial x_q} = -\frac{y_q - y}{l_q^2}, \quad \frac{\partial \theta_{pq}}{\partial y_q} = \frac{x - x_q}{l_q^2}. \] (11)

Substituting these expressions into the equilibrium conditions (9) leads to
\[ \begin{align*}
3 \sum_{i=1}^{3} (x - x_i) \left(1 - \frac{L_i}{L}\right) + \eta \sum_{pq \in S} \left(\frac{y_p - y_q}{l_p^2} - \frac{y_p - y_q}{l_q^2}\right) \Delta \theta_{pq} &= 0, \quad (12a) \\
3 \sum_{i=1}^{3} (y - y_i) \left(1 - \frac{L_i}{L}\right) - \eta \sum_{pq \in S} \left(\frac{x_p - x_q}{l_p^2} - \frac{x_p - x_q}{l_q^2}\right) \Delta \theta_{pq} &= 0. \quad (12b)
\end{align*} \]

and these equations are analytically intractable.

To make further progress, we approximate the above equations by their first order Taylor expansions in \((x, y)\) about the initial configuration \((0, L)\). Replacing each term by its Taylor series approximation leads to a linear system of 2 equations, from which the equilibrium configuration \((x, y)\) under an imposed symmetric deformation gradient \(U\) is obtained:
\[ \begin{align*}
Ax &= b. \quad (13)
\end{align*} \]

where,
\[ A_{11} = \sum_{i=1}^{3} \left(1 - \frac{L_i^2}{S_i^2}\right) - \eta \sum_{pq \in S} \left(\frac{y_p - y_q}{S_p^2} - \frac{y_p - y_q}{S_q^2}\right)^2 \\
&+ 2 \left(\frac{x_p y_p}{S_p^3} - \frac{x_q y_q}{S_q^3}\right) \Delta \theta_{pq}(0,0),
\]
\[ A_{22} = \sum_{i=1}^{3} \left(1 - \frac{L_i^2}{S_i^2}\right) - \eta \sum_{pq \in S} \left(\frac{x_p - x_q}{S_p^2} - \frac{x_p - x_q}{S_q^2}\right)^2 \\
&- 2 \left(\frac{x_p y_p}{S_p^3} - \frac{x_q y_q}{S_q^3}\right) \Delta \theta_{pq}(0,0),
\]
\[ A_{12} = A_{21} = \sum_{i=1}^{3} \left(\frac{L_i y_i}{S_i^2} + \eta \sum_{pq \in S} \left(\frac{x_p - x_q}{S_p^2} - \frac{x_p - x_q}{S_q^2}\right) \left(\frac{y_p - y_q}{S_p^2} - \frac{y_p - y_q}{S_q^2}\right) \\
&+ \left(\frac{x_p^2 y_p^2}{S_p^4} - \frac{x_q^2 y_q^2}{S_q^4}\right) \Delta \theta_{pq}(0,0),
\]
\[ b_1 = \sum_{i=1}^{3} \left(\frac{L_i}{S_i} - 1\right) + \eta \sum_{pq \in S} \left(\frac{x_p - x_q}{S_p^2} - \frac{x_p - x_q}{S_q^2}\right) \Delta \theta_{pq}(0,0),
\]
\[ b_2 = \sum_{i=1}^{3} \left(\frac{L_i}{S_i} - 1\right) - \eta \sum_{pq \in S} \left(\frac{y_p - y_q}{S_p^2} - \frac{y_p - y_q}{S_q^2}\right) \Delta \theta_{pq}(0,0).\]

From the equilibrium configuration, the energy in the unit cell is computed using Eq. (8). This strain energy describes the model completely and all key properties will be derived using this expression.

3.2. Unit cell analysis

Having derived explicit closed form analytical expressions for the equilibrium position and energy, we verify them by comparing with numerical simulations for a wide range of loading conditions and material parameters. We subject the unit cell to a symmetric deformation gradient of the form \(U\) as in Eq. (4). Fig. 4(a) displays the variation of energy for the loading case with \(\alpha = \gamma = 0\) and \(\beta\) is varied from \(-0.6\) to \(0.3\). The energy obtained from the analytical expressions are in excellent agreement with the corresponding numerical solution values for all the considered values of \(\eta\) and over the entire range of considered strains.

The response of the unit cell is considered under general loading conditions to further establish the validity of the analytical expressions. Again, only symmetric deformation gradients are considered \((R = I)\), since rigid rotations does not contribute to any energy. A general state of strain is prescribed and is characterized by the parameters \((\tilde{\alpha}, \tilde{\beta}, \tilde{\gamma})\). The components of strain are varied over a range of values \(\delta \in [-0.3, 1]\), so that the prescribed deformation gradient is
\[ F(\delta) = \left(1 + \delta \tilde{\alpha} \frac{\delta \tilde{\gamma}}{\tilde{\beta} + \delta \tilde{\gamma}}\right). \] (14)

The following loading cases are considered for comparison with numerical simulations and to illustrate the behavior of the unit cell:

- Uniaxial compression: \(\tilde{\alpha} = \tilde{\gamma} = 0\), \(\tilde{\beta} = -0.6\).
- Biaxial compression: \(\tilde{\alpha} = \tilde{\beta} = -0.3\), \(\tilde{\gamma} = 0\).
- Pure shear: \(\tilde{\alpha} = \tilde{\beta} = 0\) and \(\tilde{\gamma} = 0.5\).
- Biaxial compression with shear: \(\tilde{\alpha} = -0.2\), \(\tilde{\gamma} = 0.5\) and \(\tilde{\beta} = -0.6\).

Fig. 4(b) displays the variation of potential energy with prescribed strain for a unit cell with non-dimensional angular stiffness \(\eta = 4 \times 10^{-3}\), with \(\delta\) varied from \(-0.3\) to \(1\). The potential energy in compression changes in shape as the non-dimensional angular stiffness increases, while it maintains the same shape in tension. An excellent agreement is obtained between the analytical expressions and the numerical solutions for all other considered loading conditions over a large range of strain values, thus establishing the validity of the analytical formula for the potential energy density functional. The energy varies monotonically for the case of pure shear while it is non-convex for the other considered cases. It is monotonic in tension while there are two local minima under axial compression, corresponding to the hexagonal and re-entrant configurations when there is a component of strain in the \(y\)-direction. The strain energy is demonstrated to be non-convex and violates strong ellipticity under general loading conditions and we demonstrate in the forthcoming section that this lead to complex behaviors of finite sized lattices. Indeed, it is remarkable that our analytical expressions based on a first order approximation capture the snap-through instability and the strain energy associated with other complex loading conditions.

3.3. Equivalent stress and consistent tangent stiffness

The energy in a unit cell is a function of solely the deformation gradient \(F\) and hence the lattice can be modeled as a hyper-elastic material \((\text{Gurtin, 1982})\). The strain energy density functional \(W\) of the equivalent continuum material is assumed to be equal to the potential energy of the unit cell normalized by the cell volume \((\text{area in 2D})\) and the derivatives of this normalized energy with respect to the deformation gradient give the first Piola Kirchhoff stress \(T\) and stiffness or first elasticity tensors:
\[ \begin{align*}
T &= \frac{\partial W}{\partial F}, \quad C = \frac{\partial^2 W}{\partial F \partial F^T}. \quad (15)
\end{align*} \]
Fig. 4. Comparison of strain energy predicted by analytical solution with numerical values for (a) different values of $\eta$ under uniaxial compression and (b) different loading conditions. A good agreement is obtained for a wide range of $\eta$ across general loading conditions.

We first evaluate the energy, stress and stiffness tensors in this local coordinate system and then transform back to the global coordinate system. The tensors in the local $e_i^*$ basis are denoted by the superscript $\ast$. Note that the strain energy density $W$ is a scalar and is invariant under a change of coordinate system ($W^\ast = W$). Similarly, edge lengths $l_i$ and angles $\theta_{pq}$ are also invariant under the change of basis. For brevity, the position vectors are denoted as $x$ instead of $x^\ast$ in the following expressions. The derivatives in Eq. (15) are evaluated in a local coordinate system having a deformation gradient $U$ and the stress and stiffness tensors are given by

$$
T^\ast(U) = \frac{\partial W}{\partial F^\ast} \bigg|_{F = U}, \quad C^\ast(U) = \frac{\partial^2 W}{\partial F^\ast \partial F^\ast} \bigg|_{F = U}.
$$

Note from the above expression that, in general $T^\ast_{ij}(U) \neq T^\ast_{ij}(U)$.

The strain energy $W(F^\ast)$ is written as a function of the internal nodal coordinate $x$ (in Fig. 1(d)) and deformation gradient $F^\ast$. Noting that the internal coordinate $x$ is again a function of $F^\ast$, we write $W(F^\ast) = \mathcal{W}(F^\ast, x(F^\ast))$ and its derivative is

$$
\frac{\partial W}{\partial F^\ast} = \frac{\partial \mathcal{W}}{\partial F^\ast} + \frac{\partial \mathcal{W}}{\partial x} \left( \frac{\partial x}{\partial F^\ast} \right) = \frac{\partial \mathcal{W}}{\partial F^\ast}.
$$

where the last equality comes from the equilibrium condition on the internal nodes, thereby circumventing the evaluation of the derivative $\partial x / \partial F^\ast$. Taking the derivative of the above equation again leads to

$$
\frac{\partial^2 W}{\partial F^\ast \partial F^\ast} = \frac{\partial^2 \mathcal{W}}{\partial F^\ast \partial F^\ast} + \frac{\partial^2 \mathcal{W}}{\partial x \partial F^\ast} \left( \frac{\partial x}{\partial F^\ast} \right).
$$

(16)

The last term in the above equation can be simplified by again using the equilibrium condition. Since the equilibrium condition holds for all $F$, we have

$$
d \left( \frac{\partial \mathcal{W}}{\partial x} \right) = 0 \Rightarrow \frac{\partial^2 \mathcal{W}}{\partial F^\ast \partial x} + \frac{\partial^2 \mathcal{W}}{\partial x \partial F^\ast} \left( \frac{\partial x}{\partial F^\ast} \right) = 0.
$$
Using the above relation, Eq. (16) is now rewritten as
\[
\frac{\partial^2 W}{\partial F \partial F} = \frac{\partial^2 \tilde{W}}{\partial F \partial F} - \frac{\partial^2 \tilde{W}}{\partial F \partial \theta} \left( \frac{\partial^2 \tilde{W}}{\partial \theta \partial F} \right)^{-1} \frac{\partial^2 \tilde{W}}{\partial \theta \partial F}.
\] (17)

The above expressions can be used to explicitly determine the derivatives of the strain energy density at \( F = U \). Using the equilibrium solution Eq. (13), the first derivative is given by the explicit expression:
\[
\frac{\partial \tilde{W}}{\partial F} = \sum_{i=1}^{3} (l_i - L) \frac{\partial l_i}{\partial F} + 2\eta \sum_{pq \leq 5} \Delta \theta_{pq} \frac{\partial \theta_{pq}}{\partial F} = \sum_{i=1}^{3} (l_i - L) \left( \frac{\partial l_i}{\partial \theta_x} \frac{\partial \theta_x}{\partial F} \right) + 2\eta \sum_{pq \leq 5} \Delta \theta_{pq} \left( \frac{\partial \theta_{pq}}{\partial \theta_x} \frac{\partial \theta_x}{\partial F} + \frac{\partial \theta_{pq}}{\partial \theta_y} \frac{\partial \theta_y}{\partial F} \right).
\]

The various terms in the second derivative (17) are evaluated using the expression:
\[
\frac{\partial^2 \tilde{W}}{\partial P_l \partial P_2} = \sum_{i=1}^{3} (l_i - L) \frac{\partial^2 l_i}{\partial P_l \partial P_2} + \left( \frac{\partial l_i}{\partial P_l} \frac{\partial l_i}{\partial P_2} \right) + 2\eta \sum_{pq \leq 5} \Delta \theta_{pq} \left( \frac{\partial^{2} \theta_{pq}}{\partial P_l \partial P_2} + \frac{\partial \theta_{pq}}{\partial P_l} \frac{\partial \theta_x}{\partial P_2} + \frac{\partial \theta_{pq}}{\partial P_2} \frac{\partial \theta_x}{\partial P_l} + \frac{\partial \theta_{pq}}{\partial \theta_x} \frac{\partial \theta_x}{\partial P_l} \frac{\partial \theta_x}{\partial P_2} \right),
\]

where \( P_1 \) and \( P_2 \) can take variables \( \{x, F\} \). The expressions in Eq. (10) provide the first derivatives of \( l_i \) and \( \theta_{pq} \) with respect to \( x \), from which the second derivatives can be determined. The second derivatives with respect to \( F \) are evaluated using chain rule. For instance, the derivatives of \( \theta_{pq} \) are
\[
\frac{\partial^2 \theta_{pq}}{\partial F \partial x} = \frac{\partial \theta_{pq}}{\partial \theta_x} \frac{\partial \theta_x}{\partial F} + \frac{\partial \theta_{pq}}{\partial \theta_y} \frac{\partial \theta_y}{\partial F},
\]
\[
\frac{\partial^2 \theta_{pq}}{\partial F \partial \theta_x} = \frac{\partial \theta_{pq}}{\partial \theta_x} \frac{\partial \theta_x}{\partial F} + \frac{\partial \theta_{pq}}{\partial \theta_y} \frac{\partial \theta_y}{\partial F} + 2 \frac{\partial \theta_{pq}}{\partial \theta_x} \frac{\partial \theta_x}{\partial \theta_x} \frac{\partial \theta_x}{\partial F} + \frac{\partial^2 \theta_{pq}}{\partial \theta_x \partial \theta_y} \frac{\partial \theta_y}{\partial F},
\]
and the individual terms having the derivatives can be evaluated using Eq. (11). Finally, the derivatives of the nodes \( x_i \) are evaluated from Eq. (5). Note that the derivatives of the spatial coordinates \( x_i \) and angles \( \theta_{pq} \) with respect to the deformation gradient \( F \) in the above equations are evaluated at \( F = U \) by perturbing all the four individual components of \( U \) in Eq (4). For example, similar to the first Piola Kirchhoff stress components, we note here that in general
\[
\frac{\partial x_i}{\partial \theta_{pq}} \bigg|_{F = U} = \frac{\partial x_i}{\partial \theta_{pq}} \bigg|_{F = U}.
\]

We now derive how the stress and stiffness (first elasticity) tensors transform under a change of basis. Note that the right Cauchy Green strain tensor is invariant under a change of basis since \( C = F^T C F = U^T R^T R C F = U^T C F = C \). From material frame indifference principle (Gurtin, 1982; Jog, 2015), there exists an equivalent strain energy functional \( \tilde{W}(C) = W(F) \) and it is related to the second Piola Kirchhoff stress tensor \( S \) as \( S = 2\tilde{W}/\partial C \). Then, the first Piola Kirchhoff stress tensor in the \( \epsilon \) and \( \epsilon^* \) basis may be related as
\[
T = FS = 2F \frac{\partial \tilde{W}}{\partial C} = 2RU \frac{\partial \tilde{W}}{\partial C} = RF \left( 2 \frac{\partial \tilde{W}}{\partial C} \right) = RU^* = RT^*.
\] (18)

To derive the transformation for the stiffness tensor \( C \) under a change of basis, we note the following relation with the second elasticity tensor \( C = \partial^2 \tilde{W}/\partial C \partial C \) (Jog, 2015)
\[
C_{ijkl} = \delta_{i,j} S_{ji} + \epsilon_{im} \epsilon_{mj} R_{kj}.
\] (19)

Note that the second Piola Kirchhoff stress and second elasticity tensors are functions of \( W \) and \( C \) only and are thus invariant under a change of basis, i.e., \( S^* = S \) and \( C^* = C \) (Gurtin, 1982; Jog, 2015). Using Eq. (19), we relate the components of stiffness tensor under a change of basis as
\[
C_{ijkl}^* = \delta_{i,j} S_{ji} + \epsilon_{im} \epsilon_{mj} R_{kj}
= \delta_{i,j} S_{ji} + R_{ip} R_{jq} \epsilon_{im} \epsilon_{mj} R_{kj}
= R_{ip} \epsilon_{ij} \epsilon_{pq} + R_{ip} \epsilon_{ij} \epsilon_{pq} R_{kj}
= \epsilon_{pq} C_{pq} R_{kj}.
\] (20)

Note that we used \( R_{ip} \epsilon_{ij} \epsilon_{pq} = \delta_{ik} \) above. Finally, recalling that the \( C^* \) is the local basis, the expressions for the first Piola Kirchhoff tensor \( T \) and the stiffness tensor \( C \), given by Eqs. (18) and (20), are
\[
T_{ij} = \frac{\partial W}{\partial F} = R_{ip} \frac{\partial W}{\partial F_{ij}} \bigg|_{F = U},
\]
\[
C_{ijkl} = \frac{\partial^2 W}{\partial F_{ij} \partial F_{kl}} = R_{ip} R_{jq} \frac{\partial^2 W}{\partial F_{mj} \partial F_{ni}} \bigg|_{F = U}.
\] (22)

3.4. Variational formulation and numerical implementation

We now present the variational formulation which can be used to study the behavior of an equivalent continuum material undergoing large deformations. Consider a body occupying a domain \( \Omega \subset \mathbb{R}^3 \) in the un-deformed reference configuration, subjected to an external traction \( t \) over a part of the boundary \( \partial \Omega_t \), while displacement is prescribed over the remaining part of the boundary \( \partial \Omega_u = \partial \Omega \setminus \partial \Omega_t \). Let \( \Gamma = \{ \theta \in \mathbb{R}^3, \mathbf{v}(\theta) = 0 \ \forall \ \theta \in \partial \Omega_u \} \) be the space of test functions having zero Dirichlet boundary conditions on \( \partial \Omega_u \). The principle of virtual work is
\[
\int_{\Omega} \mathbf{v} \cdot \nabla T dV + \int_{\partial \Omega_t} \mathbf{v} \cdot (t - t_0) dS = 0 \ \forall \ \mathbf{v} \in \Gamma.
\]

Note that the integrals, gradient operator and vector \( t_0 \) are expressed in the reference configuration. Since the problem is nonlinear, an iterative procedure like Newton-Raphson is required to solve it. Let \( \mathbf{u}_k \) be the solution at the \( k \)th iteration and let \( \mathbf{u}_{k+1} = \mathbf{u}_k + \mathbf{u}_k \). Applying integration by parts, and linearizing the first term in the above principle of virtual work equation with respect to the incremental displacement \( \mathbf{u}_k \) leads to the following incremental variational formulation, which can be solved by a standard nonlinear finite element method:
\[
\int_{\Omega} \nabla \mathbf{v} : (C \nabla \mathbf{u}_k + \mathbf{T}) dV + \int_{\partial \Omega_t} \mathbf{v} \cdot (t - t_0) dS = 0 \ \forall \ \mathbf{v} \in \Gamma.
\] (23)

Bilinear isoparametric quadrilateral finite elements are used to model the domain and an inhouse finite element code is used for solving the problem. A numerical procedure similar to that used for the discrete lattice is adopted here. The boundary value problem is solved by imposing the boundary conditions in small incremental steps and using a Newton Raphson procedure at each step. At the end of each converged solution, the stiffness tensor \( C \) is checked for positive definiteness. Again, if this condition is violated and leads to a zero eigenvalue of \( C \), then the nodes are perturbed by the eigenvector corresponding to this zero eigenvalue. When a Newton Raphson procedure fails to converge, we adopt a method of steepest descent with an Armijo line search. Note that our formulation can also be incorporated into standard commercial finite element software as a user defined material.
3.5. A note on non-convex functionals

In the earlier part of this section, we observed that the lattice under study has a non-convex potential energy functional, which leads to a non-convex strain energy functional for the equivalent continuum medium. Before demonstrating the continuum behavior of the lattice, we present a brief overview of the mechanics of materials with non-convex energy functionals, which result in non-uniqueness of solutions. This non-uniqueness or bifurcation can arise both due to structural (buckling) and material instabilities and the later type of bifurcations is the focus of the present study. However, we remark here that the theoretical framework and numerical procedures used here are also applicable to structural or combined structural and material instabilities.

Typical examples include shape memory alloys (Bhattacharya, 1993) and finite deformation plasticity, where the non-uniqueness can occur either at the microscopic or the macroscopic level, and it is closely associated with the convexity property of the variational minimization problem. When the strain energy functional is not quasi-convex, the minimum energy configuration is not affine even under affine boundary conditions (Morrey, 1952), resulting in the formation of microstructural patterns that minimize the energy of the body. These patterns have been observed and studied in austenite-martensite microstructures (Ball and James, 1987), slip in single crystals (Ortiz and Repetto, 1999), kink bands in geological strata (Conti et al., 2015). These patterns arising in diverse media are characterized by layers of homogeneous deformation regions with a discontinuous gradient in the displacement field between the layers. Also, boundary layers develop at the boundary of the domain to satisfy kinematic boundary conditions. The corresponding solution may have microstructural features with infinitesimally small length scales, and a true minimizer to the continuum problem does not exist in Sobolev spaces. However, in reality, there is a natural length scale beyond which alternate energy barriers form, like bending energy (Wadee et al., 2012) and twin boundary interface energy (Arlt, 1990), preventing any further subdivision of the microstructure.

To qualify the existence and stability of an equilibrium solution under general loading conditions, several notions of generalized convexity conditions have been developed. Two key concepts in this regard are quasi-convexity and rank-one convexity of energy functionals. A functional \( \Phi \) is quasi-convex if and only if

\[
\Phi(F) \leq \frac{1}{\Omega} \int_\Omega \Phi(F + \nabla \psi) dV
\]

(24)

for all arbitrary volumes \( \Omega \), all smooth vector fields \( \psi \) with \( \psi = 0 \) on the boundary \( \partial \Omega \) and for all deformation gradients \( F \). A functional is rank-one convex if and only if \( \Phi(\lambda F_0 + (1 - \lambda) F_1) \leq \lambda \Phi(F_0) + (1 - \lambda) \Phi(F_1) \) for all \( \lambda \in [0, 1] \) and all deformation gradients \( F_0, F_1 \) such that \( \text{rank}(F_0 - F_1) \leq 1 \). A unique solution to Dirichlet boundary value problems is guaranteed if the corresponding energy functional satisfies coercivity and the sequential weak lower semi-continuity condition (swls) (Dacorogna, 2007). A quasi-convex strain energy functional satisfies swls condition and thus implies the existence of a unique solution under appropriate growth conditions. Note from the definition of quasi-convexity that the solution is affine for affine boundary conditions. On the other hand, lack of quasi-convexity can lead to microstructural patterns as solutions for minimizing the energy functional.

The effective behavior of a body having a non-quasi-convex strain energy functional is given by the quasi-convex envelope of this energy functional, a relaxed functional \( \tilde{Q}f = \sup_{\phi \in \Phi} : \phi \text{ quasi-convex} \) (Dacorogna, 2007). This envelope can be difficult to determine in practice and it is common to replace it with alternate envelopes like rank-one convex envelope. The continuum solution of the unrelaxed energy minimization problem can be represented as a weakly converging sequence of micro-structures (Dacorogna, 2007), with the strain energy in the body given by the quasi-convex envelope of the non-convex strain energy functional. The macroscopic deformed configuration can be obtained by relaxation (convexification) of the energy functional, involving simplifying assumptions and complicated numerical procedures (Carstensen, 2005), finally resulting in a solution convergent in Sobolev spaces. The corresponding effective stress is given by the derivative of this relaxed functional with respect to deformation gradient. In the present work, we do not perform any relaxation as we extract the effective macroscopic response from the finite element solution. In the next section, the lattice and the continuum medium are shown to illustrate microstructure patterns when the energy functional deviates from its rank-one convex envelope.

4. Results and discussion

To illustrate parallels between the effective behavior of the lattice and the continuum medium and to demonstrate the applicability of our homogenization procedure, we present examples under a wide range of conditions. The continuum problem is studied using finite element analysis, based on the formulation of hyperelastic material derived in the previous section. We illustrate that global patterns and micro-structures form in the discrete lattice and continuum medium, respectively, only when the strain energy functional loses rank-one convexity and does not coincide with its rank-one convex envelope at the considered deformation gradient. Assuming a separation of length scales between the lattice unit cells and the continuum finite elements, the continuum solution gives the average deformation gradient at a point in the lattice, from which the local lattice configuration can be extracted by solving for a RVE of the lattice under periodic boundary conditions (PBC). We also demonstrate that the results between the discrete and continuum medium are consistent, and the behavior of the lattice under large deformations can be potentially studied using standard isoparametric first order finite elements and the constitutive law of the homogenized model. The first three examples presented impose affine boundary conditions on a large lattice and study its effective behavior. Our final two examples involve complex non-uniform boundary conditions and deformed configurations in different parts of the lattice are captured well by the finite element solution.

We comment on some key aspects of our numerical simulations. In the lattice simulations, the solution process is stopped if at any converged solution, the masses at the opposite ends of a hexagonal cell come in contact or penetrate into the adjacent cell, since our model does not account for contacting masses. The numerical simulations are conducted over a range of torsional stiffness \( \eta \) values to demonstrate the applicability of our homogenization procedure for all values of \( \eta \). The values are chosen to highlight distinct microstructure patterns that arise under various loading conditions. Lower values of \( \eta \) produce patterns with high amplitude resulting in contacting masses. Lattices with higher \( \eta \) have patterns with low amplitudes and can go to high strains without issues like contacting masses. Our numerical procedures ensure that the solutions obtained for both the discrete and the continuum media are stable equilibrium configurations. The configurations correspond to local minimum of energy and may not be the global minimum, especially when complex micro-structures arise in the domain.

Mesh dependence of the finite element solutions is encountered in variational minimization problems beyond the onset of instability (Carstensen, 2001; Luskin, 1996). One method to resolve this mesh dependency is to use relaxed potentials
(Dacorogna, 2007; Miehe et al., 2004), as discussed in Section 3.5. In our present work using first order isoparametric elements, we obtain the effective macroscopic behavior without resorting to relaxation of the strain energy functional. Furthermore, the local deformed configuration at various points in the lattice is predicted from the continuum solution. Note that the local deformed configuration can be predicted accurately only before the onset of long wavelength instability. After the onset of this instability, the local deformed configuration of the lattice depends on the size of the domain and the lattice configurations derived from the continuum solutions are representative of the typical patterns observed in the lattice. Finally, we remark that mesh refinement in our finite element solution of the continuum model is meaningless beyond the length scale imposed by the lattice and a separation of length scales should be maintained to ensure validity of the homogenization procedure. If the loading features are small, then size dependent modeling (Kouznetsova et al., 2002) may be useful. However, we did not see the necessity for the same in the present work even when handling nonuniform and complicated boundary conditions in our numerical examples.

4.1. Uniaxial compression

4.1.1. Continuum solution: Effect of non-dimensional angular stiffness

We first demonstrate the behavior of the homogenized model by solving the equivalent continuum problem for the lattice solutions presented in Section 2.2.2. The continuum body has the same physical dimensions as the lattice in Fig. 2 and it is meshed with $10 \times 7$ finite elements. It is subjected to uniaxial compression in the $y$–direction, and a displacement boundary value problem, with an affine displacement field prescribed on all the boundary nodes, is solved to obtain the equilibrium configuration of the body. Fig. 5 illustrates the deformed configuration of the body for the strain states and stiffness parameters of the lattice in Fig. 2. The contours indicate the magnitude of compressive stress $T_{22}$ and the red (light) outline shows the un-deformed configuration. Since the lattice is subjected to uniaxial compression, the stress is uniform over the entire body and its value depends on the strain and corresponding angular stiffness $\eta$.

Figs. 5 (a)–(c) illustrate the deformed configuration for a material whose equivalent lattice has non-dimensional angular stiffness $\eta = 2 \times 10^{-2}$. The deformation field is affine for all the prescribed strains and the uniform displacement is consistent with the discrete lattice simulations in Fig. 2(c). For this value of $\eta$, the stiffness tensor derived from the strain energy functional satisfies strong ellipticity condition over the entire range of considered strains, does not exhibit any instability and the affine deformation field corresponds to the minimum energy configuration.

Figs. 5 (d)–(f) illustrate the deformed configuration for a material with non-dimensional angular stiffness parameter $\eta = 8 \times 10^{-3}$. For small strains, the deformation field is affine in the entire domain. As the strain increases, the deformation field is not affine as evident from the deformed element shapes in Fig. 5(e). As noted in Section 3.2, the functional is not rank one convex and hence is not quasi-convex. Thus, microstructural patterns form that minimize the energy of the body, subject to satisfying the kinematic boundary conditions. Fig. 5(f) displays the deformed configuration for $F_{22} = 0.6$. The deformation field is affine and it corresponds to the lattice being in the re-entrant configuration. The stiffness tensor satisfies strong ellipticity at this strain and the affine deformation field corresponds again to the minimum energy configuration of the structure.

Finally, Fig. 5(g)–(h) illustrate the deformed configuration with low non-dimensional angular stiffness parameter $\eta = 2 \times 10^{-3}$. Even at low values of strain ($F_{22} = 0.9$ in Fig. 5(g)), the deformation field is non-affine. The compressive stress is uniform throughout the domain, with minor fluctuations arising at the boundaries due to the affine prescribed displacement condition. Fig. 5(h) illustrates the non-affine deformation field at a higher strain value corresponding to $F_{22} = 0.8$. Fig. 5(i) illustrates the deformation field
at a strain value $F_{22} = 0.6$, showing that the fluctuations in displacement have decreased as the corresponding lattice attains a re-entrant configuration. Thus the finite element simulations are demonstrated to be consistent with the corresponding lattice solutions over the entire range of the considered non-dimensional angular stiffness parameters and strain values. Both media show the formation of microstructural patterns due to the loss of strong ellipticity of the Hessian of the energy functional in the transition between hexagonal and re-entrant configurations for low values of non-dimensional angular stiffness.

4.1.2. Large lattice simulation and effective behavior

Having demonstrated the typical behavior of the equivalent continuum medium for a range of non-dimensional angular stiffness, we now study the behavior of large lattices and compare with the corresponding continuum solution, obtained using a coarse finite element mesh. Consider a lattice composed of $60 \times 40$ unit cells with non-dimensional angular stiffness $\eta = 8 \times 10^{-3}$ and impose affine displacement on the boundary nodes corresponding to uniaxial compression in the $y$-direction. Fig. 6 illustrates the deformed lattice configuration at a strain level $\beta = -0.20$. Complex patterns arise in the lattice and its wavelength is sensitive to the size of the domain and the boundary conditions. We note that the wavelength of the patterns in Fig. 6 is observed to be distinct from that in Fig. 2(a), where a smaller domain resulted in a shorter wavelength. The associated instability corresponds to an infinite wavelength bifurcation mode (Geymonat et al., 1993; Triantafyllidis and Schmid, 1993). In a finite lattice, the wavelength is dictated by the size of the domain and the boundary conditions.

To compare the performance of our homogenized model in capturing the behavior of the lattice, we solve the continuum problem over the same domain, using a coarse finite element mesh. Here, a coarse mesh means the number of finite elements is much smaller than the number of unit cells in the corresponding lattice. Fig. 7(a) illustrates the deformed configuration obtained with finite element solution in a mesh of $24 \times 16$ elements at the same strain level $\beta = -0.20$. The contours display the magnitude of $T_{22}$ stress component and it has a uniform value $-2.9 \times 10^{-2}$ over the entire domain, with some minor fluctuations at the boundary. Microstructure patterns are observed in the continuum solution, similar to the patterns observed in the mesh in Fig. 5(d). As the mesh is refined further, identical patterns arise having a wavelength of two elements in the lateral direction. These patterns are thus mesh dependent and they correspond to instabilities arising due to non-convexity of the strain energy functional. Indeed, based on the discussion in Section 3.5, we remark that the continuum problem has a solution that converges only weakly to a function that does not lie in Sobolev space, the strains do not converge pointwise and the wavelength of oscillations keep decreasing with mesh refinement.

Though the deformation field is mesh dependent, the effective stress-strain response of the continuum medium is convergent under mesh refinement and matches with the corresponding lattice response. The effective stress is computed from the total energy $W$ of the numerical solution by a finite difference approximation of $T_{22} = (1/N)\partial W/\partial F_{22} = (1/N)\partial W/\partial \beta$, where $V$ is the volume of the domain. Fig. 8(a) displays this effective stress with uniaxial strain for various mesh sizes and two values of non-dimensional angular stiffness $\eta$. The bifurcation points corresponding to the onset of instability are marked in the figure. Excellent agreement is obtained between the different meshes for both values of $\eta$, well beyond the onset of instability, thus demonstrating the convergence of effective behavior of the continuum body. Fig. 8(b) displays the stress-strain response of both the lattice and the homogenized solution, along with the analytical $1 \times 1$ RVE solution. The homogenized solution is obtained using $24 \times 16$ elements while the lattice is the same as illustrated in Fig. 6. The lattice and the homogenized solutions match with the unit cell RVE solution until the point of bifurcation, which corresponds to the formation of microstructure patterns. As shown in the inset, at the onset of bifurcation, the lattice response starts to deviate from the unit cell solution. Beyond the bifurcation point, the strain energy in the domain is bounded by the quasi-convex envelope of the energy functional. The small difference between the homogenized and continuum stress-strain response beyond the point of bifurcation is attributed to finite size effects. In particular, the homogenized solution is the projection of the infinitesimal wavelength lowest energy solution onto the finite element approximation subspace, while the lattice solution has a pattern whose wavelength minimizes energy subject to compatibility with the boundary conditions. Thus, we illustrated how the homogenized solution predicts the effective lattice behavior using a FEA solution with a much coarser mesh.

The homogenized solution also predicts the deformed lattice configuration at a point. As mentioned earlier, the lattice solution at a point in the domain is obtained by extracting the deformation gradient from the continuum solution and solving for the lattice under periodic boundary conditions (PBC). Though the deformation gradient varies in the finite element solution and does not

![Fig. 6. Deformed lattice under uniaxial compression at a strain level $\beta = -0.20$. Microstructural patterns arise due to loss of strong ellipticity beyond a strain level, and their wavelength depends on the size of the domain.](image)
converge pointwise with mesh refinement, the average deformation gradient over a local region in the domain converges in the sense of Young’s measure (Bhattacharya, 2003; Dacorogna, 2007). Moreover, for a homogeneous deformation gradient prescribed at the boundary, the average deformation gradient converges to this imposed homogeneous deformation gradient at every point within the body as a consequence of minors relation (Bhattacharya, 2003).

Thus the deformation gradient at any interior point corresponds to uniaxial compression and not a combination of compression and shear, as might be construed from Fig. 7(a). The shear like patterns are oscillations due to non-convexity of the strain energy.

To get the corresponding deformed lattice configuration at an interior point in the domain, we impose this deformation gradient on a suitable RVE of the lattice with periodic boundary conditions. As mentioned earlier, the lattice instability corresponds to an infinite wavelength and a periodic domain of finite size will not match exactly the lowest energy configuration. As an example, the solution obtained on an RVE comprised of 12 × 12 unit cells subjected to uniaxial compression with PBC is illustrated in Fig. 7(b). We emphasize here that this lattice RVE solution is a stable equilibrium solution obtained by quasistatic loading with our numerical procedure and may not be a global energy minimum. As mentioned earlier, the final solution depends on the initial configuration and the loading path. Physically, it corresponds to a lattice being loaded quasistatically (slowly enough so there are no dynamic effects). Patterns similar to that in the full lattice simulations (Fig. 6) are observed in the periodic lattice. However, a careful examination shows that the wavelengths of the patterns in the two solutions do not match exactly as the discrete lattice patterns depend on the size of the finite domain and the RVE solution patterns depend on the size of the periodic domain. In our numerical simulations with PBC, patterns with larger wavelength are observed in larger RVEs and this behavior is consistent with an instability of infinite wavelength.

4.2. Shear loading

We now demonstrate the behavior of the lattice and its equivalent continuum medium under shear loading. As seen in Fig. 4(b), the strain energy is monotone along the loading direction for the pure shear loading case. Furthermore, evaluating the second derivative of the energy numerically showed it to be convex along the shear loading direction. We will now illustrate that no microstructures form when the lattice is subjected to shear deformation. For this analysis, the lattice is composed of 32 × 24 unit cells and its boundary nodes are subjected to an affine displacement field corresponding to a shear strain \( \gamma = 0.20 \). The continuum problem is solved on a domain with the same physical dimensions as the lattice, meshed with 24 × 16 elements. Fig. 9(a) and (b) illustrate, respectively, the deformation fields for the lattice and the \( T_{12} \) stress contours in the continuum medium for a material with non-dimensional angular stiffness \( \eta = 6 \times 10^{-3} \). The stress contours have a uniform value \( 2.2 \times 10^{-2} \) over the entire domain. The lattice configuration predicted by the homogenized solution, obtained by imposing the deformation gradient on a unit cell RVE with PBC, matches the displacement field observed in the lattice. Numerical simulations with other values of non-dimensional angular stiffness \( \eta \) also illustrated affine deformation fields in both.
the lattice and the continuum medium. This is indeed consistent with our assertion that micro-structures form only when the stiffness tensor violates strong ellipticity condition.

The effective stress is computed from the total energy using a finite difference approximation of $T_{12} = (1/4\partial W/\partial \gamma$. Fig. 8(b) displays the stress-strain response of the lattice and the homogenized solution, along with the analytical stress-strain variation obtained from the unit cell RVE. The response is non-linear, with the shear stiffness increasing with strain. An excellent agreement is observed between the various solutions, demonstrating the accuracy of the homogenization procedure.

4.3. Biaxial loading

The next example involves biaxial loading on a lattice having $32 \times 24$ unit cells with non-dimensional angular stiffness $\eta = 6 \times 10^{-3}$. A smaller domain is chosen so that the patterns are clearly observable. An affine displacement is imposed on the boundary nodes corresponding to the strain with $\alpha = 0.2$ and $\beta = 0.2$. As seen from Fig. 4(b), the potential energy is non-convex along the loading direction under an imposed biaxial strain. Again, for small strains, the deformation field is affine. As the strain increases, micro-structure patterns arise in the lattice, whose wavelength is sensitive to the size of the domain. Fig. 10 displays the deformed lattice configuration, with patterns which are quite distinct from that observed in the uniaxial case. Fig. 11(a) displays the corresponding homogenized solution of the equivalent continuum domain, discretized with a coarse mesh of $18 \times 12$ elements. The contours display the magnitude of $T_{11}$ stress component, which is almost uniform and equal to $-6.0 \times 10^{-2}$, with some fluctuations at the boundaries.

Micro-structures emerge in the homogenized continuum medium due to the violation of strong ellipticity condition of the stiffness tensor and they have patterns different from the uniaxial compression case observed earlier. Again, the lattice configuration at an interior point in the domain is recovered by solving for the
Fig. 9. Deformed shapes of the lattice and continuum solid subjected to uniform shear $\gamma = 0.2$. The deformation field is uniform and no microstructure patterns arise. The energy functional is convex along the shear loading direction.

Fig. 10. Deformed lattice configuration under biaxial loading with $\beta = -\alpha = 0.20$. Microstructure patterns distinct from the other cases arise due to the loss of strong ellipticity of the stiffness tensor.
lattice RVE under PBC by imposing the average deformation gradient at an interior point in the continuum body. As discussed in Section 4.1, this average deformation gradient equals the homogeneous deformation gradient imposed on the boundary. Fig. 11(b) illustrates the lattice configuration predicted by the continuum solution, obtained using a RVE composed of $12 \times 12$ unit cells, which shows features similar to that observed in the full lattice simulations. Again, similar to the uniaxial compression case, this solution is a stable equilibrium configuration and the wavelengths of the patterns are not in exact agreement with the full lattice simulation. Furthermore, as the RVE size is increased, the wavelength of the patterns also increases, demonstrating that the stable configuration has infinite wavelength. The continuum solution predicts the existence of instabilities in the lattice. However, like in the uniaxial compression case, its exact configuration depends on the boundary conditions and on the size of the domain.

4.4. Flat punch problem

To further illustrate the applicability of our homogenized model, we consider a problem where displacement is prescribed on part of the boundary. A lattice having $60 \times 40$ unit cells with non-dimensional angular stiffness $\eta = 6 \times 10^{-3}$ is considered, with rollers placed on the sides and the bottom surface. A constant displacement is prescribed on the center one-third of the top surface, while the remaining part is traction free.

Fig. 12 (a) illustrates the deformed configuration of the lattice at a displacement $d = 0.25H$, where $H$ is the height of the domain. The deformation patterns are observed to vary throughout the domain. The corresponding homogenized problem is solved with a finite element mesh of $24 \times 16$ elements. Fig. 12(b) illustrates the finite element solution of the deformed configuration along with the $T_{22}$ stress contours at the same prescribed displacement value. Also shown are the lattice configurations at four locations in the contin-
uum domain. These lattice configurations are obtained solving an RVE with $5 \times 5$ unit cells under PBC by imposing the deformation gradient extracted from the FEA solution at these four locations. When there is no instability, the lattice configuration predicted by the RVE does not depend on its size and a $1 \times 1$ RVE can be used. An RVE composed of $5 \times 5$ unit cells is used to clearly display the lattice configuration, even if there are no instability patterns. When a long wavelength instability arises in the lattice, the patterns depend on the RVE size. As discussed earlier, in such cases, only a qualitative comparison of the deformed lattice configurations is possible. The lattice configurations predicted by the homogenized solution are in agreement with those observed in the full lattice simulations in Fig. 12(a), thus illustrating the validity of our homogenization procedure.

The variation of the external force acting on the punch region with prescribed displacement $d$ is calculated from the total energy $E$ in the domain by a finite difference approximation of $F = \partial E / \partial d$. Fig. 13(a) displays the force displacement response for both the lattice and continuum solutions, with the displacement normalized by $H$. A good agreement is observed between the two solutions, with the small mismatch arising due to boundary effects. Fig. 13(b) displays the same force displacement data for various mesh sizes.
along with the finite lattice solution. Good results are obtained even with coarse meshes and the accuracy improves as the mesh is refined. The finite element solution for the 48 × 32 mesh failed to converge beyond $d = 0.2H$ as the mesh gets highly distorted near the region where the corner of the punch contacts the body and the element volumes become negative.

4.5. Double punch problem

Our final example involves subjecting the lattice to extreme deformations by a double punch. The lattice has the same physical dimensions and non-dimensional angular stiffness as in the previous example in Section 4.4. Consider a coordinate system with the origin located at the lower left corner of the domain and let $x, L$ and $H$ denote the horizontal coordinate, length and height of the domain, respectively. The center one-third of the top and bottom surfaces are subjected to the displacement field $f(x) = 25H(x/L - 0.2)(x/L - 0.8)/9$ at the top surface and $-f(x)$ at the bottom surface. The remainder of the top and bottom surfaces are traction free and rollers are placed along the sides. The problem is solved by imposing the displacement in steps and using a Newton Raphson solution procedure. The displacement imposed at any step is $\rho f(x)$ and $\rho$ is increased in steps from 0 to 1. Fig. 14(a) illustrates the deformed lattice showing a complex pattern forming between the displacement prescribed regions, while the deformation is less away from these regions. Zoomed-in views of the deformed lattice at four distinct points illustrate the wide range of deformation gradients in the domain.

Fig. 14 (b) illustrates the deformed configuration of the corresponding homogenized continuum solution on a $24 \times 16$ finite element mesh along with the $T_{22}$ stress contours. It also displays the lattice configuration predicted by the homogenized solution at the corresponding points as shown for the lattice in Fig. 14(a). Good agreement between the discrete lattice and homogenized solution is obtained for the deformed configurations at various points. The second mode of instability is observed in the deformation zone.
Fig. 14. Deformed configurations of (a) the lattice and (b) its corresponding continuum domain, with the inset shows the lattice deformation patterns predicted by the homogenized solution at a point. Instabilities form in a part of the lattice and they are captured accurately by the homogenized solution.

Let \( d \) be the maximum value of \( \rho f(x) \) (displacement of the center of the bottom surface) at each solution step. A measure of the force acting on the displacement prescribed regions is calculated using \( F = \partial E / \partial d \). This force is evaluated by finite differencing using the energy at each solution step (force at step \( i \) is \( F_i = (E_i - E_{i-1})/(d_i - d_{i-1}) \)). Fig. 13(a) displays the force displacement response of both the lattice and the continuum solutions. The response is close to bilinear, with the corner corresponding to the onset of instability. The small mismatch between the homogenized and lattice solutions is attributed to effects at the boundary, where the homogenization procedure is not expected to be effective. A good agreement is observed between the two solutions, thus illustrating the effectiveness of our homogenization procedure in capturing the effective behavior of large lattices with a much coarser finite element mesh.

5. Conclusions

This paper investigates the large deformation behavior of hexagonal lattices. In the first part of the work, a bistable lattice transforming from the hexagonal to the re-entrant configuration is
studied using a unit cell. The lattice is modeled by linear axial and angular springs, with nonlinearity coming solely from large deformation geometric effects. Analytical expressions for the strain energy in a unit cell are derived under an arbitrary prescribed deformation gradient and are found to be in excellent agreement with numerical simulations. The strain energy is shown to deviate from its rank-one convex envelope for lattices with non-dimensional angular stiffness below a threshold value. Next, the lattice is modeled as a continuum hyper-elastic material and its constitutive law is derived from the lattice potential energy functional. The strain energy functional of this equivalent continuum material is not quasiconvex. By analyzing the energy landscape of a single unit cell of the lattice, we are able to predict bifurcations. Furthermore, since there are multiple local minima in the energy functional, we draw analogies between the lattice deformations and phase mixtures observed in shape memory alloys and shear bands in finite deformation plasticity.

In the second part, simulations on large lattices and their corresponding continuum medium are performed under a wide range of loading conditions to demonstrate the ability of the developed continuum model to predict the lattice behavior. The lattice forms microstructure patterns having wavelengths of the order of domain size. The corresponding finite element solutions also exhibit mesh dependent pattern formations, arising due to the non-convexity of strain energy. The formation of these patterns and the effective stress-strain response of the lattice are captured accurately by the homogenized solution. Complex loading conditions are considered in our final two examples, where the homogenized solution captures the effective deformation of the lattice. Furthermore, the force-displacement response is also predicted accurately by the homogenized solution using coarse finite element meshes, thus demonstrating the applicability of the model under general loading conditions. When long wavelength bifurcations occur, though the lattice displacement patterns depend on the domain size and boundary conditions, the effective macroscopic behavior (force-displacement or stress-strain response) can be extracted from the macroscopic continuum model even after the onset of bifurcation.

We finally remark on some possible future directions of our work. This paper illustrates the possibility of relating the microstructure features observed in finite plasticity, shape memory alloys, deformation patterns in rocks with the patterns in finite lattices, which incorporate a natural length scale. An explicit relation between the two may allow modeling of large lattices with the finite element techniques developed for continuum medium which involve complex micro-structures and require relaxation of the energy functional. For example, the effect of dynamic loading on the localized lattice deformations can be addressed to design reconfigurable lattices.

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