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A continuum model for nonlinear lattices under large deformations

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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.

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 (Keating, 1966) to truss structures (Wadley et al., 2003) to granular media (Cundall and Strack, 1979). In recent years, focus has been placed on designing tailored lattices for attaining specific objectives (Evans et al., 2001) such as lightweight, heat dissipation and multifunctionality. There have primarily been two approaches for modeling lattices. The first approach, pioneered by Gibson et al. (1982); Gibson and Ashby (1997), models lattice materials as slender beams and has been applied extensively to study two-dimensional (2*D*) 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 (Kirkwood, 1939) has been extensively used, for example, to study properties of polymer molecules (Tasumi et al., 1962), atomic lattices (Rücker and Methfessel, 1995), and percolation in elastic media (Kantor and Webman, 1984).

Buckling and instabilities arising in lattices undergoing large deformations have been extensively studied. Ohno et al. (2002) 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. Triantafyllidis and coworkers (Geymonat et al., 1993; Triantafyllidis and Bardenhagen, 1996; Triantafyllidis and Schnaidt, 1993; Triantafyllidis and Schraad, 1998) applied Bloch analysis to investigate the onset of bifurcation by examining the tangent stiffness matrix of a unit cell representative volume element (RVE). A number of approaches (Vigliotti and Pasini, 2012; 2013) have been developed for homogenization of lattices to determine their effective mechanical properties at the continuum level. Asada et al. (2009); Okumura et al. (2004) developed a two-scale homogenization procedure to study microscopic buckling and post-buckling behavior of periodic elastoplastic cellular solids, Tadmor et al. (1999) developed homogenization of three-dimensional (3*D*) atomic lattices with convex potentials to derive bulk properties and behavior of materials. Arroyo and Belytschko (2002) 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, (Arroyo and Arias, 2008) 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. Miehe et al. (2002) developed a homogenization procedure for periodic composites undergoing large deformations and exhibiting both structural (buckling) and material (due to non-convexity) instabilities.

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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 homogeneous deformation 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 a subject of recent interest due to their suitability for the development of diverse engineering applications, including tunable metamaterials (Schaeffer 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 (1*D*) 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 2*D* 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 $\pi/2$ and is termed re-entrant when atleast one interior angle is less than $\pi/2$. 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 2*D* 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 axial and angular stiffness, denoted k_a and k_t, 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 θ^i_{pq} between the edges is related to the degrees of freedom by the kinematic relation:

$$\cos(\theta^i_{pq}) = \frac{(\mathbf{x}_i - \mathbf{x}_j, \mathbf{x}_i - \mathbf{x}_k)}{|\mathbf{x}_i - \mathbf{x}_j||\mathbf{x}_i - \mathbf{x}_k|}, \tag{1}$$

where (., .) and |.| denote, respectively, the scalar product and *l*2 norm of the vectors. Let $\Delta\theta^i_{pq}$ denote the change in this angle between edges (*p, q*) and let ΔL^m_{ij} be the change in length of an axial spring on edge *m* connecting nodes *i* and *j*, expressed as:

$$\Delta L^m_{ij} = |\mathbf{x}_i - \mathbf{x}_j| - L. \tag{2}$$

The potential energy of the lattice is given by

$$E = E_a + E_t = \sum_{m=1}^{N} \frac{1}{2} k_a (\Delta L^m_{ij})^2 + \sum_{i=1}^{M} \sum_{e=p,q} \frac{1}{2} k_t (\Delta\theta^i_{pq})^2, \tag{3}$$

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*,