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Wiggly strain localizations in peridynamic bars with non-convex potential

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ABSTRACT

We discuss the static states of a peridynamic nonlinear elastic bar of finite length in a hard device, which represents a continuum description of a complex hierarchical structure with interacting long-range crosslinkers, of the type encountered in biological systems. The nonlocal character of the model requires that edge conditions are defined on a boundary layer with the same length of the horizon, affecting the solution in the bulk interior. Assuming that the constituent microscopic ligaments contain bistable units governed by a non-convex potential, we show that the development of coexisting folded-unfolded phases, either synchronized or unsynchronized, induces in the displacement field the formation of undulations at a micro-scale of the length of the horizon, associated with strain localizations triggered at the bar ends. The equilibrium paths, found numerically with a pseudo-arc-length continuation method, become unstable within a certain range of elongation, suggesting the possible occurrence of a negative-stiffness response.

1. Introduction

The response of a wide range of different-in-type materials to strain- or stress-induced disturbances is governed by an underlying microscopic transition in a great variety of configurations. Diffusionless martensitic transformation and twinning are associated with fine layered microstructures in phase transforming materials (Ball and James, 1987; Bhattacharya, 1992). When ductile solids are deformed into the plastic range, the deformation highly localizes in slip bands, progressively forming and almost equally spaced, usually following the directions of maximum shear (Froli and Royer-Carfagni, 1999). Strain localization in the form of shear bands may also represent the preferential pre-failure deformation mode of natural rocks, granular materials and quasi-brittle materials in general (Amitrano and Schmittbuhl, 2002). In all these cases, the typical stress-strain relation shows a mismatch between the nucleation and the propagation thresholds, due to a nucleation peak possibly accompanied by nonlocal interactions between phases, slip bands, or cracks.

To simulate phenomena of this kind, the absolute minimization of a non (quasi) convex elastic energy for the material has represented for the last decades a far reaching approach that generalizes, for the solid state, the van der Waals model for fluids. This has become clear since Ericksen's analysis (Ericksen, 1975) of the equilibrium of finite-length bars pulled at the ends governed by a non-monotonic stress-strain constitutive relation. This is characterized through the local and global minimizers of a free energy functional of the form

$$\mathcal{E}[u] = \int_{x=0}^{L} \Phi(u')\, dx\,, \tag{1.1}$$

complemented by the work done by external forces in the case of a soft device. In (1.1) $x \in (0, L)$ is the position of a material point of the bar in its natural state, $u : (0, L) \to \mathbb{R}$ and $u'\,(0, L) \to \mathbb{R}$ are, respectively, the displacement field and its spatial derivative, and Φ is the strain energy density, which is non-covex from the assumed form of the constitutive relation. At certain values of the average elongation, there exists an uncountable number of inhomogeneous, energy-minimizing equilibrium solutions for the bar, showing that, albeit the above indeterminacy, nonlinear elasticity theory can model phase transitions and the formation of equilibrium mixtures in solid bodies. Several attempts have been made to reduce the indeterminacy and predict the location of interfaces across which the displacement gradients are discontinuous (see,

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e.g., Vainchtein et al., 1999 and references cited therein). The basic strategy has been to add terms on the right-hand-side of (1.1), to penalize the formation of sharp interfaces and control their number, so to capture the formation of finite-scale microstructures, phase nucleation and hysteresis (Vainchtein et al., 1999). Recently, Xuan et al. (2015) have used this model together with a hybrid numerical method to calculate approximate inhomogeneous solutions, characterized by the interface number, interface thickness and strain amplitude.

An application of non-convex minimization to describe the phenomena of strain localization and serrated deformation of mild steel was pursued in Royer-Carfagni (2000). Supposing that the energy density $\Phi(\cdot)$ is a function not of the local strain u' but of its average weighted value over a reference length, the model could explain the onset of elastic, plastic and strain-hardening phases in a bar, interpreting the formation of slip bands and stress oscillations (Portevin–Le Chatelier effect). The model was later extended in De-Lellis and Royer-Carfagni (2002) by adding a surface energy term, but keeping as a distinctive feature the nonlocal spatial dependence of the strain measure. Indeed, in the orderly formation of plastic bands in tensile bars, as evidenced in the experimental campaign of Froli and Royer-Carfagni (1999), the crucial role is played by the nonlocal interaction of particles, that in Froli and Royer-Carfagni (2000) has been interpreted through a 1D assembly of interacting links.

We believe that the peridynamic theory represents a powerful tool to interpret phenomena of this kind, for which phase-like transformation and nonlocal effects are decisive. Developed independently by Kunin (1982, 1983), Rogula (1982), and Silling (2000) and further generalized in Silling et al. (2007), the peridynamic theory is an extension of the classical continuum mechanics theory, in which the differential operator is replaced by integrals of interaction forces between near particles separated by finite distances within an intrinsic material length, called the *horizon*. Since then, several models have been proposed, among which the linear peridynamic model proposed in Aguiar and Fosdick (2014) and (Aguiar, 2016a; 2016b), which is a generalization of a linearized peridynamic approach of Silling et al. (2007).

The combination of the peridynamic idea with non-convex minimization appears to have been first explored by Dayal and Bhattacharya (2006) to study the kinetics of phase transformations. The material model for the interaction forces has a non-monotonic trilinear form, in analogy with the non-monotonic stress-strain relation of Ericksen's bars, and a viscous damping term. The authors used a particular measure of "*strain*" (sometimes called *elongation*) in their constitutive relation, defined as $\delta u/\delta x$, where $\delta x = x' - x$ is the signed distance between particles at x' and x, whereas $\delta u = u(x') - u(x)$ is the corresponding relative displacement. In the static case, the corresponding equilibrium equation would be of the form

$$\int_{x=0}^{L} \phi\left(\frac{\delta u}{\delta x}\right) h(\delta x)\, d x + b(x) = 0\,, \tag{1.2}$$

where, apart from a possible viscous damping term, $\phi(\cdot)$ is a non-monotone trilinear function, $h(\cdot)$ is a function decaying rapidly and $b(x)$ denotes the body force *per* unit reference length. In this way, any jump in the displacement field provokes a singularity in this measure of strain ($\delta u \not\to 0$ as $\delta x \to 0$), which is energetically penalized. As a consequence of this, the response of the bar in a hard device has similarities with Ericksen's model: the material leaves the low-strain curve close to the Maxwell stress, suffers strain increments at constant stress till it reaches the high-strain curve and then follows it (see Dayal and Bhattacharya, 2006, Section 4). The phase boundaries nucleate at the ends of the bar and move along the bar as the applied displacement increases. Due to the intrinsic nonlocal character of peridynamics, no additional conditions, such as nucleation criterion and kinetic relations, are needed to simulate phase boundary nucleation and propagation.

Here, we also use a non-monotone relation and a local stability criterium to perform a detailed investigation of the morphology of microstructures and phase mixtures, but the basic difference between our approach and that of Dayal and Bhattacharya (2006) is that, here, the trilinear constitutive equation is a function of the relative displacement δu only, *not* weighted by $1/\delta x$ as in (1.2). This provokes a "weak" interaction between neighboring points, so that *strain localizations* may easily appear. Since the major strength of the peridynamic theory is that it can be applied on highly irregular fields, it is worth investigating models of this type, which represent the nonlinear extension of the cases considered in Silling et al. (2003) and Mikata (2012).

The proposed model may represent the hierarchical network architecture of complex distributed biological systems. Representative examples are skeletal muscles, whose response at fast time scales is dominated by long range interactions that induce cooperative behavior of the constituent ligaments (Caruel et al., 2013), or proteins, which have been modeled as elastically bonded network amenable of mechanical unfolding in different pulling directions (Dietz and Rief, 2008). Further examples are the unzipping of biological macromolecules studied by Gupta et al. (2011) and the folding and unfolding of RNA hairpins analyzed by Thomas and Imafuku (2012) using a conventional zipping model that includes both the free energy for RNA binding and the elastic free energy of the system. Approaches of this kind aim at simulating that the cells of multicellular organisms adhere to the extracellular matrix through clusters, spanning a size range from very few to thousands of adhesion bonds.

With reference to the paradigmatic case of striated muscles, Huxley and Simmons (1971) suggested that each cross linker be represented by a hard spin model, with a bistable potential providing two folding configurations, assumed to have infinitely narrow energy wells corresponding to two distinct chemical states. A snap-spring element can be alternatively used, to remove the irregularities driven by the hard spin model and effectively interpolate between the soft and hard device behaviors (Marcucci and Truskinovsky, 2010; Caruel et al., 2015). Such element may be further complemented with a series spring, to simulate the connection with the back bone in the case of muscles, or the elasticity of the filaments in the case of proteins (Dietz and Rief, 2008). When elements of this kind are arranged in complex bundles, the overall response may correspond to synchronized phase transitions, where the individual units undergo conformal changes, interpreted as generic unfolding states in the bistable elements. This may lead to unusual material properties, such as negative equilibrium stiffness and different behavior in force- and displacement-controlled loading conditions (Caruel et al., 2015).

There are cases for which experiments indicate that the elastic coupling modeled by the series spring is not significant (Dietz and Rief, 2008), so that the response of the single cross link is governed by the spin element only. Here, we assume a regular arrangement of cross links with different size ranges, whose response is a function of the relative displacement of the link ends. The continuum description of this arrangement is a perydinamic bar, where the properties of the spin elements are modeled through snap-springs, active within the horizon and tuned by the material micromodulus. This model allows for *discontinuous* displacement fields, which may be associated with the occurrence of strain localizations, fractures, or, plastic slips.

The nonlinear peridynamic model can capture interface number, interface thickness, and strain amplitude, but the resulting microstructure becomes really very complex due to the nonlinear nonlocal interactions. Three stages of deformation are identified. The first stage, called *undulation*, corresponds to oscillations in the