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Quasiconvex envelopes of energies for nematic elastomers in the small strain regime and applications

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ABSTRACT

We provide some explicit formulas for the quasiconvex envelope of energy densities for nematic elastomers in the small strain regime and plane strain conditions. We then demonstrate their use as a powerful tool for the interpretation of mechanical experiments. Analytical formulas characterizing the stress–strain response in pure shear are derived, providing an easily testable benchmark for future numerical and experimental investigations on the mechanics of nematic elastomers.

1. Introduction: nematic elastomers

Nematic elastomers are polymeric materials with embedded nematic mesogens. Their mechanical response is governed by the coupling of rubber elasticity with the orientational order of a liquid crystalline phase. Nematic elastomers exhibit large spontaneous deformations, which can be triggered and controlled by many different means (temperature, electric fields, irradiation by UV light). These properties make them interesting as materials for fast soft actuators and justify the considerable attention that they have attracted in recent years. The reader is referred to the monograph by Warner and Terentjev (2007) for a thorough introduction to the physics of nematic elastomers, and for an extensive list of references.

While commercial applications exploiting their properties are still lacking, nematic elastomers are playing an important role as a model system for the study of the mechanics of phase transforming materials. In these materials, because of the symmetries of the phase transformation underlying their unusual mechanical properties, material instabilities are ubiquitous. Seen from the point of view of hyperelasticity, this means that the energy densities capable of reproducing the elastic response of phase transforming materials lack the convexity properties necessary to guarantee material stability. On the other hand, recent advances in the Calculus of Variations allow us to show that suitable convex envelopes of the energy densities (the so-called quasiconvex envelopes) may provide valuable insight on the mechanical response of these materials. These techniques have been applied with considerable success in a variety of physical systems including nematic elastomers, shape memory alloys, magnetostrictive or ferroelectric materials, crystal plasticity (see Bhattacharya, 2003 for a review). In this paper, we

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apply this approach to nematic elastomers in the small strain regime (geometrically linear theory), restricting our attention to plane strain conditions for simplicity.

The main new findings reported in this paper are the following. First, we obtain a new relaxation result leading to an explicit formula for the quasiconvex envelope of an anisotropic energy density proposed to model nematic elastomers within the framework of geometrically linear theories, in plane strain conditions. This result, illustrated in Section 3 and proved in the Appendix, extends to the anisotropic case techniques employed in Cesana (2010) to analyze isotropic energy densities. As observed already in Biggins et al. (2008) and DeSimone and Teresi (2009), the use of anisotropic energies is crucial to avoid that imposed stretches may be accommodated at zero stress (ideally soft response), and to obtain results in agreement with the available experimental evidence (in particular, non-vanishing shear moduli in the natural state of the material, see Rogez et al., 2006).

Second, we obtain an explicit analytical characterization for the stress–strain response of a sample of nematic elastomer tested in pure shear. The key tool used for this purpose is the new explicit formula for the quasiconvex envelope of the energy density, as explained in Section 4. In fact, we use the quasiconvex envelope to obtain the energy of a sample responding to the applied loads through deformations that are macroscopically homogeneous, but are spatially modulated at small length scales by systems of shear bands (usually called stripe domains in the nematic elastomer literature, see Verwey et al., 1996; Finkelmann et al., 1997). This leads to an explicit expression of the elastic energy stored in the sample, as a function of the prescribed elongation. We then obtain the stress–strain response by straightforward differentiation.

The mechanical significance of our results can be summarized as follows. First, through the explicit analytical representation of the stress–strain response in pure shear, we provide a new, easily testable benchmark that may prove useful in future numerical and experimental investigations on the mechanics of nematic elastomers. Second, we are now able to discuss the relationship between the energies and quasiconvex envelopes of the geometrically linear theory with their counterparts in the fully nonlinear theory, and to understand the impact of anisotropy. The availability of explicit formulas in both regimes is a rather unique feature of nematic elastomers, and a fortunate circumstance. We find that the insight on the geometric structure of the energy landscape deriving from the possibility of comparing them against each other (and with experiments, thanks to the new results on anisotropic energies) is particularly enlightening.

While the geometrically linear theory has obvious limitations (see, e.g., Bhattacharya, 2003), it is a very valuable conceptual tool in the study of phase transforming materials. It is simpler in many (though not all) respects, it is familiar to larger groups of users, the resulting energy landscape has an easier geometric structure, rigorous mathematical results available for it (some of which are first proved in this paper) are more complete (see Cesana, 2010; Cesana and DeSimone, 2009). Most importantly, the linear theory lends itself more easily to the exploration of model extensions such as, for example, accounting for the effects of applied electric fields, including curvature elasticity terms typical of liquid crystals, modeling rate effects and viscous relaxation to equilibrium. All these are easily handled by simply adding new terms in the governing energy and by introducing appropriate dissipation potentials (see, e.g., Fukunaga et al., 2008). By contrast, exploring deeply nonlinear regimes may require more complex coupling schemes. In all these extensions, the insight on energetically optimal states deriving from the explicit knowledge of the quasiconvex envelope of the elastic energy density proves to be a very valuable tool.

The rest of the paper is organized as follows. In Section 2 we recall some model energy densities for nematic elastomers, introduce the notion of quasiconvex envelope, and illustrate it by comparing two corresponding isotropic expressions arising from the geometrically linear and the fully nonlinear theory. In Section 3 we consider plane strain conditions, and discuss the new formula for the quasiconvex envelope of an anisotropic energy density. The formula is then applied in Section 4, where we simulate some of the experiments that can be used to probe the mechanical properties of nematic elastomers.

The paper is written in the language of Continuum Mechanics. We have included also rigorous proofs of our results, which require some familiarity with advanced tools from the Calculus of Variations. This more mathematical part is contained in two Appendices, which can be skipped by readers wishing to concentrate only on the physical significance of our results and on their implications on the mechanical response of nematic elastomers. Parts of this material, such as the lamination construction contained in Proposition 4 of Section Appendix B, are however very useful to gain a deeper understanding of the material instabilities which make the mechanical response of nematic elastomers so interesting.

2. Energies and their quasiconvex envelopes

Following DeSimone and Teresi (2009), we are interested in three model expressions for the energy density of a nematic elastomer in the small strain regime (geometrically linear theory). The first one is

$$\tilde{\Phi}(\mathbf{E},\mathbf{n}) = \mu|\mathbf{E}_d - \mathbf{E}_0(\mathbf{n})|^2 + \tfrac{1}{2}\kappa(\mathrm{tr}\,\mathbf{E})^2, \tag{1}$$

where $\mathbf{E}_d = \mathbf{E} - \frac{1}{3}\mathrm{tr}(\mathbf{E})\mathbf{I}$ is the deviatoric part of the infinitesimal strain $\mathbf{E}$,

$$\mathbf{E}_0(\mathbf{n}) = \frac{3}{2}\gamma\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbf{I}\right) \tag{2}$$