Modeling liquid crystal elastomers: actuators, pumps, and robots

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ABSTRACT

We model the dynamics of shape evolution of liquid crystal elastomers (LCE) in three dimensions using finite element elastodynamics. The model predicts the macroscopic mechanical response induced by changes in nematic order, e.g. by heating or cooling through the isotropic/nematic transition or, in azo-doped materials, by exposure to light. We model the performance of LCE actuator devices including multicomponent actuators, peristaltic pumps and self-propelled robots. The goal of this work is to build a bridge between basic soft matter theory and practical materials engineering/device design. Supported by NSF-DMR-0605889.

Keywords: Liquid crystal elastomer, nematic, phase transition, actuator, finite element, simulation, azobenzene, photoisomerization

1. INTRODUCTION

Soft materials can undergo shape changes under a variety of stimuli including temperature changes, applied electric and magnetic fields, optical illumination, mechanical stresses, and changes in solvent conditions. An important example is liquid crystal elastomers (LCE's), a novel class of materials with potential applications as soft actuators, also known as "artificial muscles[1-11]." While piezoelectric hard materials typically produce strains of order 1%, liquid crystal elastomers can show induced strains up to 400% and induced bending up to ± 70° [7-9]. Compared to hard materials, elastomers offer the advantage of being flexible and thus more fracture-resistant. For these reasons there is great motivation to develop liquid crystal elastomers as soft actuators for engineering applications.

We consider here the special case of nematic elastomers. These materials are crosslinked polymer networks covalently bonded to long, rigid, liquid-crystalline mesogens.[1] In the low temperature nematic phase, the mesogens show long-range orientational order, while above the isotropic-nematic (I-N) transition, orientational order disappears and the material becomes isotropic. Accompanying this phase transition is a change of shape. On heating through the I-N transition, a monodomain sample shrinks along the axis parallel to the nematic director and expands along the two transverse axes, reminiscent of the contraction of a muscle. LCE's doped with azo-dyes can also be actuated by illumination[7-9]. Here, dye molecules change from elongated to bent molecular shape upon absorption of light, thus disrupting orientational order.

The mechanics of nematic LCE's are thus controlled by intrinsic coupling between nematic order and mechanical strain. Theoretical models of this coupling can be solved analytically, e.g. if the goal is to predict the mechanical response of a representative volume element, as described at length in [1] and references therein. The goal of the present work, however, is more ambitious: we wish to model entire devices containing LCE actuators and simulate their behavior on laboratory length and time scales, including dynamics as well as static response, in three dimensions. Geometries and boundary conditions of interest are not simple enough to allow for analytical solutions, so we turn to finite element simulation methods to simulate the elastodynamics. Finite element methods have been used previously to model 2-d statics of LCE's[12,13] but have not, to our knowledge, previously been used to model dynamics in 3-d.

Instead of using a preconfigured software package, we have developed our own finite element simulation code based on a Hamiltonian approach. Our algorithm is based on a marvelously simple approach to finite element elastodynamics proposed by Broughton et al[14]. However Broughton's algorithm relies on the approximation that both strain and rotation are small, and their finite element Hamiltonian is not invariant under rotation. As a result, dynamics calculated from such a Hamiltonian conserve energy poorly particularly in the case of finite rotations. As a solution to this difficulty, we replace the linear strain tensor in Broughton's approach with the Green-Lagrange strain tensor, a measure of deformation that is invariant under sample rotation, containing both linear and nonlinear terms. This substitution renders our Hamiltonian rotationally invariant and thus our algorithm is not limited to the small-rotation limit. The resulting

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dynamics show remarkable numerical stability, and total energy and momentum are both conserved to high precision. Details of the algorithm will be published elsewhere[15].

2. MODEL

We model a nematic elastomer by discretizing its volume into a mesh of tetrahedral elements. The potential energy per unit volume within each tetrahedral element is written as

$$U_{potential} = \frac{1}{2} C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} - s Q_{ij} \varepsilon_{ij} \qquad (1)$$

Here ε_{ij} is the Green-Lagrange strain tensor, C_{ijkl} represents the stiffness tensor associated with the material, and Q_{ij} is the nematic order tensor. The coupling constant s is a material parameter that specifies the strength of the coupling between nematic order and strain, controlling for instance how much an aligned monodomain sample will change length in the isotropic-nematic transition. We note that since the Green-Lagrange strain ε_{ij} is defined in the material or body frame, we must also define C_{ijkl} and Q_{ij} in the body frame. Thus if the sample undergoes a rotation, these quantities conveniently rotate with the body rather than being defined in the lab frame.

To construct a Hamiltonian we also need to specify the kinetic energy of the system. Here we follow the method used by Broughton et al[14] and apply the "lumped mass" approximation, which assumes that all the mass is concentrated in the nodes of the finite element mesh.

In our simulation, the initial position and velocity of each node in the material are specified in the initial state. The subsequent dynamics of the system are calculated explicitly using a finite time step. After each Δt, the potential energy in (1) is calculated for each element as a function of the corner nodes' displacements from their initial, relaxed positions. Forces on each node are calculated as a derivative of the total potential energy in all adjacent volume elements with respect to the node's position. The node positions and velocities are then updated using the velocity Verlet method.

This finite element explicit dynamics algorithm closely resembles the familiar molecular dynamics method and is almost as easy to code. Here we are moving nodes rather than atoms, and instead of an interatomic potential we are using the potential energy in (1), expressed as a function of node displacements. Full details will be provided in [15].

The next question is how to consider the time evolution of the nematic order tensor Q_{ij}. In the present work we start with the simple approximation that we can externally control the state of nematic order. For instance if we cool (heat) the sample through the isotropic/nematic transition, we increase (decrease) of the nematic order throughout the entire body, respectively. Alternatively, if we shine light on a sample of an azo-doped material, we reduce nematic order only in a thin surface region where the light is absorbed. So here we consider the response of the strain to changes in nematic order which we control externally. In future work we will also consider the natural dynamics of Q_{ij}, for instance to observe the nucleation and evolution of orientational domains.

Dissipation in the elastomer is modeled in the form of forces acting between adjacent nodes in the mesh with magnitude proportional to the local velocity gradient. This simple isotropic form preserves conservation of momentum and angular momentum. Anisotropic dissipation will be included in future versions of the model.

In setting up the simulation, we can apply point constraints; e.g. by anchoring one or more surface nodes, we can effectively "glue" one edge of the sample to a supporting surface. Alternatively we can add extra terms to the model to represent kinetic and static friction between surface nodes and a nearby bounding surface such as a floor. Gravitational or other external forces can also be added.

3. APPLICATIONS

3.1 Actuators

In [8], Camacho-Lopez et al demonstrated that an azo-doped liquid crystal elastomer beam anchored on one edge bends spontaneously when illuminated on one side. Here we model the mechanical response of such a system. In Figure 1 (left) we show a beam in its initial nematic state with its director aligned horizontally. Then we switch the top layer of the sample, shown in red, from nematic to isotropic, by setting the nematic order tensor Q_{ij} to zero only within volume elements on the top of the sample. The resulting surface contraction induces a rapid bend, pulling the beam into a curved

position as shown in Figure 1. The resulting radius of curvature depends on many variables including the thickness and elastic properties of the beam; the strength of the nematic-strain coupling; the magnitude of the reduction in the nematic-order parameter in the surface layer; and the thickness of the surface layer. The time response of the beam depends also on the kinetics of the *trans-cis* photoisomerization of azobenzene chromophores in the material.

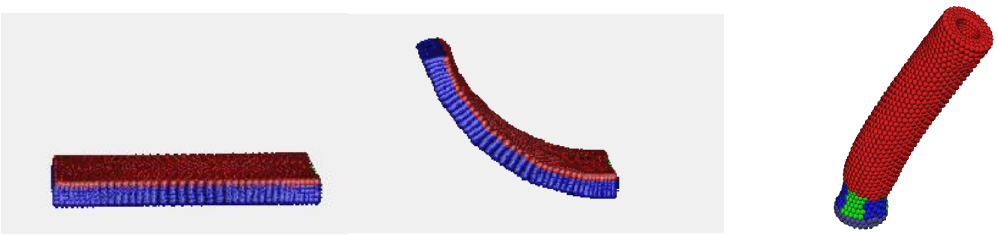


Fig. 1. Finite element simulations—An azo-doped nematic elastomer beam anchored on its right edge spontaneously bends upward when illuminated from above; modeling an experiment by Camacho-Lopez et al [8]. Left: the beam before illumination, entirely in the nematic state with the director oriented horizontally. Middle: the top (red) layer is switched to isotropic, inducing rapid upward bend. Right: A red rubber tube is oriented by the motion of six nematic elastomer actuators (shown in blue and green) arrayed in a ring at the tube's base.

Also shown in Fig. 1 is a more complex geometry in which a hollow rubber tube is oriented by the action of six nematic elastomer actuators embedded in the tube walls at its base. Each actuator may be extended or contracted individually, and can thus hold the tube fixed at a chosen orientation or else whirl it around in a circular motion.

3.2 Peristaltic Pump

Because of their exceptional ability to change shape and mimic the behavior of muscles, nematic elastomers are a good candidate for engineering of peristaltic pumps. Peristalsis is the process by which propagating undulation in a tube or channel induces motion of its contents. This is for example the mechanism by which food is transported through the human digestive system.

We have modeled two highly idealized conceptual designs for peristaltic pumps composed of nematic elastomers. The first of these is a tube-shaped structure with the nematic director oriented along the tube's long axis. To induce a propagating wave, we apply a modulation to the strength of the scalar nematic order parameter along the length of the tube with a selected wavelength and frequency. Such modulation could be created e.g. by non-uniform heating or by a pattern of laser illumination switched on/off periodically along the tube to create a moving wave. Such a device might be useful for transport of highly viscous fluids or slurries. A second configuration is also shown; here we induce a similar propagating oscillation in a thin film designed to cover a rigid channel and move the fluid inside. Alternatively a pair of such films might be used on opposite sides of a channel.

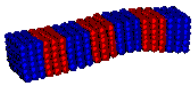
Fig. 2. Finite element simulation—Left: A nematic elastomer tube undulates in a peristaltic motion, induced by periodic modulation of the scalar nematic order parameter along its length, e.g. by temperature or light. Nodes of the finite element mesh as visualized as spheres. This simulation includes 4885 nodes and 19,352 tetrahedral volume elements. Right: We model peristaltic motion in a thin film designed to cover a rigid channel and transport its contents. Alternatively two parallel walls of a channel could be made to undulate this way to drive fluid flow.

3.3 Soft, self-propelled robot

Earthworms move by a propagating wave of muscle contraction, alternately shortening and lengthening the body along its length. This motion can be replicated in a nematic elastomer by applying a modulation in the magnitude of the nematic order parameter, much as in the pumps modeled above.

To enable motion of the center of mass, an earthworm also needs friction with a nearby surface. The underside of a real earthworm is decorated with tiny bristles (setae) that allow it to anchor one section of the body while another section is in motion. To mimic this behavior we could also imagine placing bristles on the underside of a nematic elastomer earthworm robot. Alternatively, asymmetric static friction can be created by suitable surface morphology on the substrate. For instance, an elongated monodomain nematic elastomer film can be made to "crawl" by placing it on an asymmetric substrate, e.g. on brushed velvet. Local contraction and elongation can be induced by moving a heat source just above the film from one end to the other.

In our nematic elastomer "earthworm" simulation, shown in Video 1, we apply perfect asymmetric static friction so that the simulated earthworm can slide forwards but cannot slide backwards. Kinetic friction is also included with a finite friction coefficient.



Video 1: Finite element simulation—A nematic elastomer contracts and elongates, mimicking the motion of an earthworm as it crawls over hilly terrain. http://dx.doi.org/10.1117/12.768282.1

4. DISCUSSION

This work represents an important first step in modeling shape change in nematic elastomer devices because it allows prediction of material response in complex geometries, looking not only at statics but at dynamics in three dimensions. Our immediate goal in developing this modeling approach is to accelerate engineering of devices whose motion is driven by nematic elastomers, and to explore ideas, even in highly idealized form, for the dvelopment of novel technologies based on LCE's. In the future, we anticipate that our finite element approach will be useful for simulating a wide range of soft materials that may undergo large deformations, e.g. in response to changes in orientational order.

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