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Morphing Liquid Crystal Elastomer Coatings: A Machine Learning Approach to Inverse Design

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Liquid Crystal Elastomers (LCE) undergo programmable shape-morphing in response to a change of temperature, illumination, or other stimulus. The resulting trajectory is programmed by patterning the nematic director field. A key challenge in LCE device engineering is the inverse design problem: find the nematic director field that morphs a sample to a complex desired target shape e.g. when heated. Inspired by our recent collaboration with the Lavrentovich group [1], we investigate the inverse design problem for LCE surface coatings that morph to form complex topographies. We present a novel machine learning approach to address this inverse design challenge. First, we solve 1500 "forward" problems via fast finite element methods [2] for various director configurations to form a training dataset. Next, we train a stacked ensemble regression model using the Autogluon framework [3]. Here 80% of the dataset was used to train the models including tree-based and deep learning algorithms. The prediction of the two parameters defining the director field on the remaining test dataset was evaluated. The ensemble model outperformed any individual model and could also predict configurations that departed from the initial geometry by adding noise. As an example we model the design of morphing LCE suction cups to mimic the gripping capabilities of octopus suckers. We discuss plans to extend this approach to a broader class of LCE device geometries.

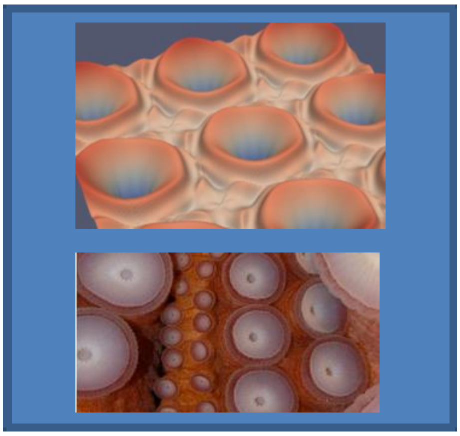

Figure 1—(Top) FEM simulation studies of LCE suction cups that morph from a flat coating on stimulus, inspired by (bottom) octopus suckers. (Photo by Steve Lodefink, Wikimedia Commons.)

In addition we address an unrelated but equally fundamental topic in nematic liquid crystals: heterogeneous disclination loop nucleation via the Frank-Read source mechanism. Using a materials-by-design approach, we propose that a liquid crystal cell with a patterned array of Frank-Read sources will demonstrate a rheological response that depends on disclination half-loop sizes, density, orientation, and pattern. Defect half-loops pinned on colloids with planar anchoring may also serve as Frank-Read sources. We discuss the importance of this mechanism in rheology of both passive and active nematics.

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