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COMPUTATIONAL MODELING OF RESPONSIVE NEMATIC ELASTOMERS

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Nematic elastomers are highly deformable polymers showing non-symmetric elasticity, provided by their capability to show a reversible phase transition between the isotropic to the transversally istotropic (nematic) phase. The above-mentioned phase transition, triggered by environmental stimuli whose nature depends on the chemistry of the material (such as heat, light, magnetic field, etc.), can be harnessed to obtain a macroscopic detectable deformation making the material responsive [1]-[3].

In the present study, we consider the nematic-isotropic phase transition occurring in Liquid Crystal Elastomers (LCE), a family of elastomers possessing rigid mesogens linked to the material's backbone chain network whose arrangment in space can be easily controlled by a temperature variation [4]. The development of LCE materials with a polydomain structure, i.e. characterized by an architected pattern of organized mesogen units arrangments, allows obtaining a wide range of actuation capabilities.

Starting from the statistical-based molecular mechanics of polymers, we illustrate the main governing equations of the mechanics of LCEs and their computational implementation in a finite element (FE) framework. The nematic to isotropic phase transition is assumed to occur when the so-called transition temperature T_{NI} of the material is overcome (Figure 1).

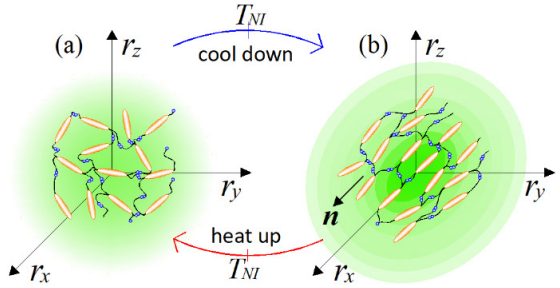

Figure 1. - Reversible isotropic (a)-nematic(b) network transition in LCEs upon a temperature change

Several examples, demonstrating the responsive capabilities of this class of materials where the mesogens arrangment is properly set, are illustrated and discussed.

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