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Mesoscopic modelling and size effect for the mechanics of multi-walled carbon nanotubes

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ABSTRACT

We propose to model thick multiwalled carbon nanotubes (MCNTS) as beams with non-convex curvature energy. Such models develop stressed phase mixtures composed of smoothly bent sections and rippled sections [1]. This model is motivated by experimental observations and large-scale atomistic-based simulations[2,3,4]. The model is analyzed, validated against large-scale simulations, and exercised in examples of interest. It is shown that modelling MWCNTs as linear elastic beams can result in poor approximations that overestimate the elastic restoring force considerably, particularly for thick tubes. In contrast, the proposed model produces very accurate predictions both of the restoring force and of the phase pattern. We characterize through large-scale simulations the nonlinear elastic response of MWNCNTs in torsion (see Fig.1) and bending [5]. We identify a unified law consisting of two distinct power-law regimes in the energy-deformation relation. This law encapsulates the complex nonlinear mechanics of rippling and is described in terms of elastic constants, a critical length-scale and an anharmonic energy-deformation exponent. The mechanical response of MWCNTs is found to be strongly size-dependent, in that the critical strain beyond which they behave nonlinearly scales as the inverse of their diameter. These predictions agree with available experimental observations.

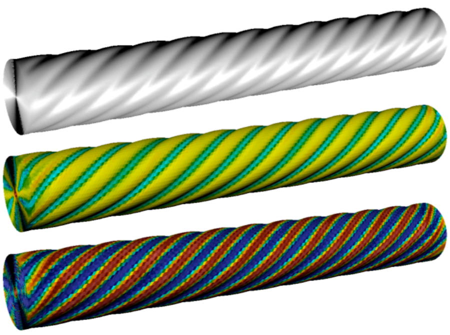

Figure: Typical torsion simulation of a 40-walled carbon nanotube

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