Multiwalled carbon nanotubes: the thicker, the softer

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Size matters for the mechanics of multiwalled carbon nanotubes (MWCNTs). It has been known for some time that MWCNTs often wrinkle under deformation exhibiting the so-called rippling deformation pattern, which makes MWCNTs much softer. Through large-scale multiscale simulations [1-3] we have characterized with a power law the softer wrinkled response, and showed that the transition strain between the super-stiff behaviour attributed to MWCNTs and this softer regime scales as the inverse of the tube diameter [4]. Thus, the tera Pascal Young's modulus can be fully exploited in devices and materials with for moderately sized MWCNTs or tubes subject to moderate deformations. Similarly, in interpreting experiments or designing devices, the classical Euler-Bernouilli beam theory can only be applied to such tubes.

The elasticity of thick MWCNTs is nonlinear. These tubes typically display mixtures of wrinkled and unwrinkled sections, and often exhibit hysteretic mechanical behaviour. This makes thick MWCNTs attractive components for energy dissipation. We propose to model thick multiwalled carbon nanotubes as beams with non-convex curvature energy [5]. Such models develop stressed phase mixtures composed of smoothly bent sections and rippled sections. This model is motivated by experimental observations and large-scale atomistic-based simulations. 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.

References:

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Figures:

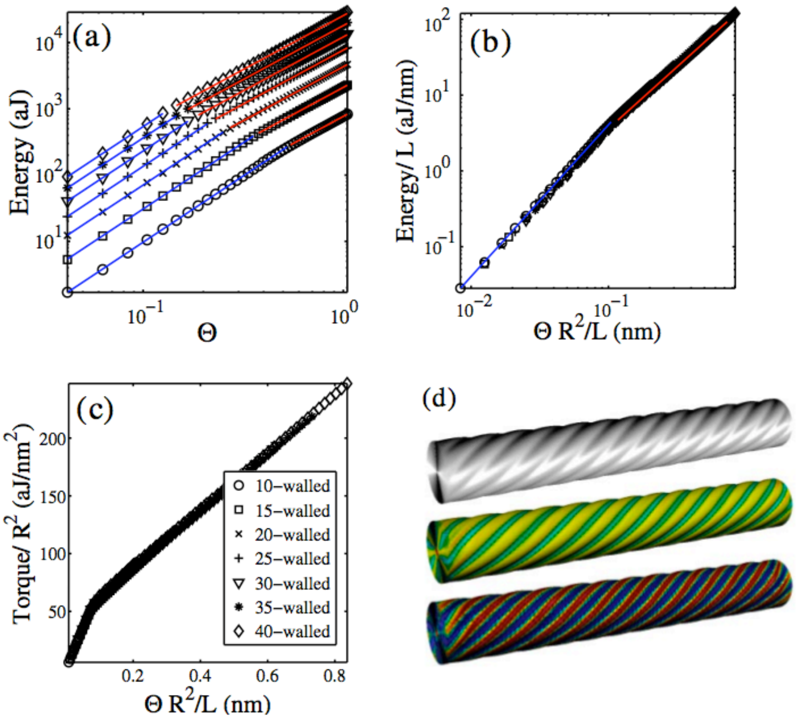

Figure 1: Twisted MWCNTs. (a) Strain energy vs twisting angle log-log plots for various MWCNTs and (b) data collapse upon appropriate rescaling. The power-law fits with exponents 2 (blue) and 1.63 (red) are shown for illustration. (c) Rescaled torque vs twisting angle relation highlighting the unified law. (d) 35-walled CNT in torsion, deformed shape (top), Gaussian curvature map (middle, green is zero, red is positive, blue is negative), and energy density map (bottom, red is high, blue is low).

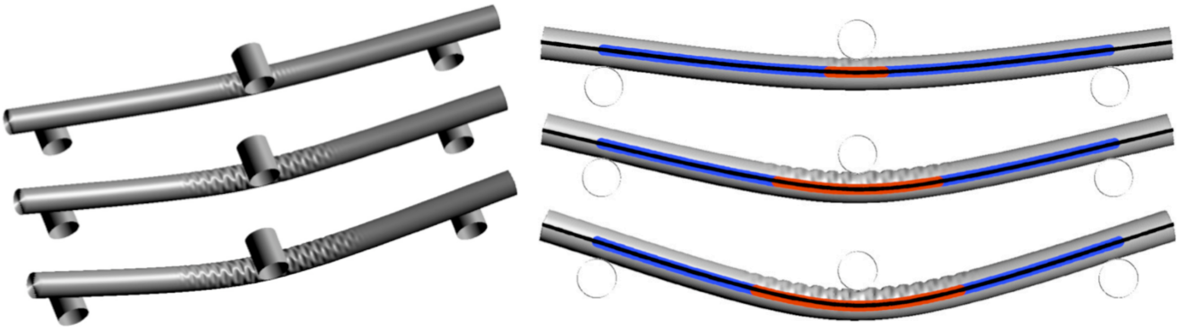

Figure 2: View of the 3D deformation of a 20-walled CNT 280 nm long subjected to a vertical displacement of 28 nm, from the onset of rippling to the last computed configuration (left). Comparison between the deformations and rippling patterns provided by the full 3D model and the mesoscopic beam model (right).

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