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Shape transitions in bistable carbon nanotubes coupled to encapsulated gas OLEG SHKLYAEV, ERIC MOCKENSTURM, MILTON COLE, VINCENT CRESPI, The Pennsylvania State University — Large-diameter single-wall carbon nanotubes are bistable (i.e. can have inflated or collapsed cross-sections) and can be used to design nano-electromechanical systems such as engines, generators, and heat pumps. The underlying physical mechanism for these devices is the sensitivity of the tube's equilibrium shape to external stimuli such as temperature and applied voltage. Fixing one end in the inflated state and the other in the collapsed state creates a mobile transition region separating these states. Gas encapsulated inside the tube provides an additional means to control the tube shape by coupling its thermodynamic parameters to the equilibrium tube configuration. Depending on the conditions, the encapsulated gas can remain vapor or condense layer-by-layer on the inner wall surface. We analyze such a system with lattice-gas model and molecular dynamics simulations. Changing the gas temperature or number of gas atoms changes the relative fraction of collapsed and inflated regions, while external forces that change the tube shape also affect the phase of the encapsulated gas. Surprisingly, squashing an inflated tube that has gas condensed on its inner surface decreases the surface area available to the wetting layer, so that gas atoms are forced back into the vapor phase: a paradoxical effect where compression induces a transition from condensed to vapor phases.

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