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Effective Shear Strain in Helical Rippled Carbon Nanotubes: A Unifying Concept for Understanding Electromechanical Response TRAIAN DUMITRICA, DONG-BO ZHANG, University of Minnesota — Despite its importance, little is known about how complex deformation modes alter the intrinsic electronic states of carbon nanotubes. Here we consider the rippling deformation mode characterized by helicoidal furrows and ridges and elucidate that a new intralayer strain effect rather than the known bilayer coupling and σ-π orbital mixing effects dominates its gapping. When an effective shear strain is used, it is possible to link both the electrical and the mechanical response of the complex rippled morphology to the known behavior of cylindrical tubes. In combination with objective molecular dynamics, this concept may be useful for understanding the electromechanical characteristics of large scale carbon nanotube assemblies and other individual nanoscale forms of carbon.
Reference: D.-B. Zhang and T. Dumitrică, ACS Nano (2010) DOI: 10.1021/nn1019658.

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