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Dislocation Onset and Glide in Carbon Nanotubes under Torsion

TRAIAN DUMITRICA, DONG-BO ZHANG, RICHARD JAMES, University of Minnesota — The torsional plastic response of carbon nanotubes is comprehensively described in the objective molecular dynamics framework [1-3]. It is shown that an (n,m) tube is prone to slip along a nearly-axial helical path, which introduces a distinct (+1,-1) change in the wrapping index. The low energy realization occurs without loss of mass, via nucleation of a 5-7-7-5 dislocation dipole, followed by a nearly-axial glide of the 5-7 dislocation. The onset of plasticity depends not only on chirality but also on handedness. For a given handedness of the applied twist, chiral tubes of opposed handedness are most susceptible to yield. A right-handed applied twist on an armchair (zig-zag) tube leads to a right- (left-) handed tube.

[1] T. Dumitrică and R.D. James, *Objective Molecular Dynamics*, Journal of the Mechanics and Physics of Solids **55**, 2206 (2007).
[2] D.-B. Zhang, M. Hua, and T. Dumitrică, *Stability of Polycrystalline and Wurtzite Si Nanowires via Symmetry-Adapted Tight-Binding Objective Molecular Dynamics*, Journal of Chemical Physics **128**, 084104 (2008).
[3] D.-B. Zhang and T. Dumitrică, *Elasticity of Ideal Single-Walled Carbon Nanotubes via Symmetry-Adapted Tight-Binding Objective Modeling*, Applied Physics Letters **93**, 031919 (2008).

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