

Abstract Submitted
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Pull out instability in double walled carbon nanocones ARINDAM RAJ, Material Science and Engineering, Indian Inst of Tech-Kanpur, SHAKTI S GUPTA, Mechanical Engineering, Indian Inst of Tech-Kanpur, DEEPTI VERMA, Department of Chemical Engineering and Materials Science, University of Minnesota — Here, we present a molecular mechanics (MM) based study to show sharp changes in the variation of potential energy and wall morphology in double walled carbon nanocones (DWCNCs), when the constituent cones are pulled away from each other. In the MM simulations, bonded and non-bonded interactions among carbon atoms are prescribed using MM3 potential. The process of pulling out is simulated by constraining the base atoms of an inner cone and incrementally moving the tip atoms of the outer cone in the coaxial direction. In the relaxed state DWCNCs, the wall to wall normal distance between the cones is found to be 3.4\AA , consistent with that obtained in two-layered graphene sheets. For each incremental step of separation, the minimum energy configuration of the entire system is obtained and the associated potential energy recorded. The instability leads to loss of concentricity of the cross-sections of cones in the sense that the wall of the outer cone deforms, making a single-sided cam-lobe type structure. DWCNCs of two different apex angles show the pull-out instability at almost the same separation distance.

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