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Carbon Nanotubes under Hydrostatic Pressure: The Deformation Transition MARVIN L. COHEN, CATALIN D. SPATARU, STEVEN G. LOUIE, U. C. Berkeley and LBNL, RODRIGO B. CAPAZ, Universidade Federal do Rio de Janeiro, PAUL TANGNEY, The Molecular Foundry, LBNL — Isolated single-wall carbon nanotubes (SWNTs) deform from their usual cylindrical shape to a collapsed or oval cross-section upon increase of hydrostatic pressure. We use classical molecular-dynamics simulations to study the structural properties of isolated SWNTs under pressure near this deformation transition. Within our model, we find two distinct behaviors depending on the nanotube diameter d. For $d > d_c \approx 12$ Å, SWNTs collapse from a circle to a peanut or racetrack cross-section at a critical pressure P_c with a discontinuous change in volume. The van der Waals interactions between the opposite walls of the tube play a crucial role in driving this discontinuous transition. For a range of pressures, both circle and collapsed cross-sections are locally stable and the system shows hysteresis. For $d < d_c$, the transition is continuous, from a circle to an oval cross-section. RBC acknowledges financial support from the John Simon Guggenheim Memorial Foundation and Brazilian funding agencies CNPq, CAPES, FAPERJ, Instituto de Nanociências, FUJB-UFRJ and PRONEX-MCT. This work was supported by NSF Grant No. DMR04-39768 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. DOE under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NERSC and NPACI.

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