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A Failure Criterion for Single-Walled Carbon Nanotubes Based on Molecular Mechanics ANTONIO AVILA[1], Univesidade Federal de Minas Gerais, GUILHERME LACERDA, Universidade Federal de Minas Gerais — Single-walled carbon nanotubes (SWNT) are the natural choice for high performance materials. The problem, however, rises when the experimental data are compared against each other. The large variability of experimental data lead to development of a new set of numerical simulations called molecular mechanics, which is a "symbiotic" association of molecular dynamics and solid mechanics. This papers deals with a molecular mechanics simulations of single-walled carbon nanotubes. Three SWNT configurations and its combinations were simulated, i.e. armchair, zigzag and chiral. The failure criterion introduced is based on modified Morse's potential with dissociation energy of 124 Kcal/mol and an inflection point considered is around 13% of strain. The numerical data are in good agreement with data from Belytschko et al. (2002) where the failure occurred at 10.6% strain at 65.2 GPa of stress. To be able to identify the highest stress concentration region, one end of the SWNT all degrees-of-freedom were fixed and a prescribed axial displacement was applied at the opposite end. The Sadoc (chiral-chiral) configuration had the highest stress at the smallest chiral SWNT. For the Dunlap configuration (chiral-zigzag) the highest stress occurred at chiral part close to the pentagon location.

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