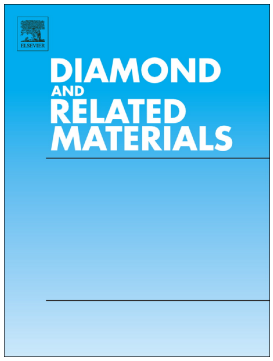

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An Investigation on Tensile Properties of Coiled Carbon Nanotubes Using Molecular Dynamics Simulation

E. Shahini [a], K. Karimi Taheri [b], A. Karimi Taheri [a,*]

[a] Department of Material Science and Engineering, Sharif University of Technology, Azadi Ave. Tehran, Iran, PO Box: 11155-9466

[b] Mechanical and Industrial Engineering Department, Northeastern University, Boston, MA o2115, USA

Abstract

A coiled carbon nanotube (CCNT) can be formed from the distortion of parent toroidal carbon nanotube with a uniform pitch length and a uniform spring rise angle. In this research molecular dynamics simulation was carried out to assess the tensile properties of three CCNT having indexes of (3,3), (4,4), and (5,5). The results indicated that Stone-Wales defects are necessary for thermodynamic stability of the CCNTs. The stress-strain curves showed that the yield stress, yield strain, and failure strain are decreased with increase in temperature. The force-displacement curves revealed that the spring constant of these materials is highly depended on the tube diameter and rising angle, while it is not noticeably depended on temperature. However, the toughness of the (4,4) CCNT at different temperatures and rising angles indicated that the CCNT has the highest toughness at lower temperatures and rising angles. Also, it was shown that a (4,4) CCNT presents its largest toughness at temperature of 100 K and the rising angle of 12.5 degrees.

Keywords: Carbon nanotubes; Molecular dynamics simulation; Mechanical behavior; Tension test

[*]Corresponding author. Tel: +982166165220. E-mail: ktaheri@sharif.edu (Ali Karimi Taheri)