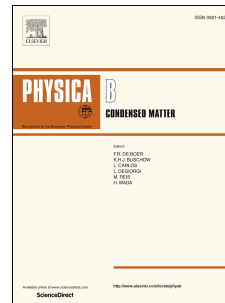


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Seyed Mostafa Rahimian-Koloor, Seyed Majid Hashemianzadeh, Mahmood M. Shokrieh



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Effect of CNT Structural Defects on the Mechanical Properties of CNT/Epoxy Nanocomposite

Seyed Mostafa Rahimian-Kolour^a, Seyed Majid Hashemianzadeh^{a,*}, Mahmood M. Shokrieh^b

^aMolecular Simulation Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran, 16746-13114, Iran

^bComposites Research Laboratory, Center of Excellence in Experimental Solid Mechanics and Dynamics, School of Mechanical Engineering, Iran University of Science and Technology, Tehran, 16846-13114, Iran

*Corresponding Author: Tel: +98-21-77240287, E-mail: Hashemianzadeh@iust.ac.ir

Abstract

The mechanical behavior of epoxy-based nanocomposite in the presence of pristine single wall carbon nanotube (SWCNT) and the SWCNTs including Thrown-Stone-Wales and vacancy defects has been studied using non-equilibrium molecular dynamics simulation and the density functional theory calculations. The continuous SWCNT as a long nanofiber has been considered to construct the nanocomposite representative volume element. In this respect, an in-situ curing process was performed using the LAMMPS software and an in-house code. The results indicated that despite the enhancement of longitudinal and transverse Young's moduli, the shear moduli of the nanocomposite with the pristine SWCNT were reduced compared to the pure polymer. It was shown that although the presence of defects reduces the elastic properties of isolated SWCNTs, they improve the nanocomposite properties. To explain these findings, the influence of defects on the structural integrity of nanocomposite and interfacial bonding strength has been investigated.

Keywords: CNT/Epoxy Nanocomposite; Mechanical property; Defect; MD Simulation; Curing; Pullout

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