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S. Sahmani, A.M. Fattahi



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Calibration of developed nonlocal anisotropic shear deformable plate model for uniaxial instability of 3D metallic carbon nanosheets using MD simulations

S. Sahmani ^{a*}, A.M. Fattahi ^b

^a *Department of Mechanical Engineering, Bandar Anzali Branch, Islamic Azad University, Bandar Anzali, Iran*

^b *Department of Mechanical Engineering, Tabriz Branch, Islamic Azad University, Tabriz, Iran*

Abstract

In comparison with semiconducting carbon structures, the metallic carbon exhibits more novel properties due to their high density of states as well as superconductivity. As a result, prediction of mechanical properties associated with three-dimensional (3D) carbon structures is very attractive. In this paper, the size-dependent nonlinear uniaxial instability of 3D metallic carbon nanosheets containing interlocking hexagonal carbon bonds is investigated based on a novel calibrated nonlocal anisotropic plate model. To accomplish this purpose, Eringen's nonlocal continuum elasticity is incorporated to an exponential shear deformation plate theory. To extract the proper value of nonlocal parameter, the critical buckling loads and associated postbuckling equilibrium curves obtained by the established size-dependent plate model are compared with those of molecular dynamics (MD) simulations corresponding to various nanosheet side lengths and different boundary conditions. It is displayed that the calibrated nonlocal plate model with the proposed proper value of nonlocal parameter equal to 1.12 nm for fully simply supported edge supports and 1.26 nm for fully clamped edge supports has a very good capability to anticipate accurately both of the buckling and postbuckling characteristic of the uniaxially loaded 3D metallic carbon nanosheets.

Keywords: Carbon nanostructure; Metallicity; Nonlocal continuum elasticity; Nonlinear buckling; Molecular dynamics simulation.

1. Introduction

Because of unique physical and mechanical characteristics of families of carbon nanostructures, a new foundation to apply more efficient materials in different emerging fields of nanoscience and nanotechnology have been created. In recent years, several new types of carbon-based allotropes have

*Corresponding author. Tel.: +98 21 66405844, Fax: +98 21 66419736.

E-mail addresses: sahmani@gmail.com; sahmani@aut.ac.ir (S. Sahmani).

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