عنوان مقاله:

Analysis of Nonlinear Mechanical Response of Coiled Carbon Nanotubes under Axial Loading Using Molecular Mechanics Finite Element Method

محل انتشار:

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نویسندگان:

Seyed Hadi GHADERI - Department of Mechanical Engineering, Shahrood University of Technology

Ehsan HAJIESMAILI - Department of Mechanical Engineering, Shahrood University of Technology

خلاصه مقاله:

In this paper, mechanical response of single-walled helically coiled carbon nanotubes (CCNTs) under large axial compression and elongation is studied using an atomistic based finite element method. A systematic approach is adopted to construct the atomistic structure of CCNTs which is to determine the reference configuration of the CCNTs. The CCNTs are stretched until failure and compressed until onset of buckling or until the adjacent coils touch each other. The relationship between the applied displacement and the reaction force is investigated, the spring constants of CCNTs are calculated over the entire loading range and the strain dependency of spring constant is discussed. The variation of the stiffness of an individual CCNT is found to be controlled by the changes in the interatomic bond stiffness and the geometry of CCNT during axial deformation. The fracture of these nanostructures under tensile force is studied. The most interesting observations are the superelasticity, buckling under compression, and brittle fracture of CCNTs in tension.

کلمات کلیدی:

Coiled carbon nanotube, Molecular mechanics finite element method (MMFEM), Spring constant, Large deformations