Torsional Fracture Pattern of Carbon Nanotube Bundles: A Reactive Molecular Dynamics Study

Tainá de Sousa Oliveira[1], Marcelo Lopes Pereira Júnior[2], Luiz Antônio Ribeiro Júnior[1]

[1]University of Brasília (*Institute of Physics*) , [2]University of Brasília (*Faculty of Technology*)

e-mail: tainaoliveiraif@outlook.com

Carbon nanotubes (CNTs) have received increasing attention from the scientific community in recent years due to the numerous properties that surpass those of any material known so far. CNTs present interesting mechanical properties, because they are very resistant and flexible, besides having high thermal and electrical conduction, which enables their application in several areas. There is a technological race to manufacture this material on an industrial scale, but some limitations need to be overcome, showing the need for constant research to understand the mechanisms involved in these materials, according to the desired application. Here, reactive computational molecular dynamics simulations were performed to study the mechanical strength and fracture pattern of CNT bundles (CNTBs) from the systematic torsion of one of their edges. The CNTBs considered here are made up of seven carbon nanotubes, six of which are arranged in a hexagonal configuration, and one central nanotube. To perform the simulations, we used the open-source software LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), with ReaxFF (Reactive Force Field) potential. The study was done with CNTs of different diameters (~4 and ~18 Å) and chiralities (armchair, zigzag and chiral). Our results indicate that the fracture patterns of the CNTBs are diameter dependent, and that the armchair-type CNTBs proved to be more resistant. On the other hand, smaller diameter CNTBs proved to be stronger than larger diameter ones, due to their greater stability. A result of great importance is that torsion in CNTBs formed by CNTs with smaller diameters leads to nanodiamandoid formation in the fracture region.

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References:

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