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Numerical Simulations Defect-Decorated Carbon Nanotubes under Pressure

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Carbon nanotubes (CNTs) are amongst the strongest materials known with very high tensile strength and Young's modulus. Unfortunately the ideal parameters primarily refer to single nanotubes. In amorphous materials and non-twisted bundles the macroscopic strength is limited by the relatively weak van der Waals interaction between the tubes.
In recent years researchers have tried to modify CNT-based materials in various ways, including irradiation to create defect-decorated CNTs. In this paper we present Density Functional Theory and Molecular Dynamics simulations of defect-decorated CNTs. We show that even small fractions of extra defects in the material can lower the collapse pressures significantly. The extra defects also facilitate deformations into oval and race-track shapes at lower pressures. The interplay between defect-decorations and pressures further allows for local morphological changes, including CNT-interlinking, which do not lessen the strength of CNTs further, but might improve other material properties.

Apply to be considered for a student ; award (Yes / No)?

No

Level for award;(Hons, MSc, PhD, N/A)?

N/A

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