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Abstract

Mechanical strengthening of composite materials that include carbon nanotubes (CNT) requires strong inter-bonding to achieve significant CNT-CNT or CNT-matrix load transfer. The same principle is applicable to the improvement of CNT bundles and calls for covalent crosslinks between individual tubes. In this work, sulfur crosslinks are studied using a combination of density functional theory (DFT) and classical molecular dynamics (MD). Atomic chains of at least two sulfur atoms or more are shown to be stable between both zigzag and armchair CNTs. All types of crosslinked CNTs exhibit significantly improved load transfer. Moreover, sulfur crosslinks show evidence of a cooperative self-healing mechanism allowing for links to rebond once broken leading to sustained load transfer under shear loading. Additionally, a general approach for utilizing machine learning for assessing the ground state electron density is developed and applied to these sulfur crosslinked CNTs.

Introduction

Strong and lightweight are materials goal that have become sought after in many applications. These factors are especially important in the development of next-generation aerospace vehicles where weight is already a limiting factor in low Earth orbit launches and becomes increasingly critical as the range of the flight increases.[1] Aerodynamic and engine e□ciencies are already suitable for several conceptual missions; these missions are impossible with current structural materials. Since their discovery, the use of carbon nanotubes (CNTs) as mechanical reinforcement agents was highly anticipated due to their tremendous strength and