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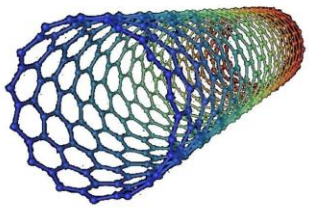
MOLECULAR DYNAMICS SIMULATION OF INTERFACIAL BONDING PROPERTIES OF CARBON NANOTUBE REINFORCED COMPOSITES

Keywords: Sustainable technologies, Density Functional Theory, molecular modeling, reactive force fields

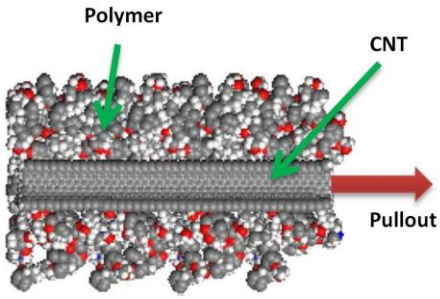
In collaboration with the research group Mechanics of Materials and Structures (UGent)

Composite materials play an important role in modern engineering. Aerospace, automotive, and many other industries replace the traditional metallic materials with new advanced composites. For instance, fiber reinforced composite materials make up 25% of the A380's airframe, by weight. Among the different reinforcements, carbon nanotubes are used increasingly in advanced composites. Their excellent mechanical and thermal properties make them a versatile reinforcement for composites. In recent years, many researchers have studied mechanical properties of nanotube reinforced polymer composites. These studies revealed that incorporating a few percentages of carbon nanotubes could improve the flexural and tensile strengths, hardness, wear resistance, electrical and thermal properties of polymer composites.

Goal Interfacial bonding is one of the most fundamental issues in the study and development of carbon nanotube (CNT) reinforced polymer composites. The interfacial bonding characteristics determine the load transfer capability from polymer matrix to nanotube. The objective of this study is to perform molecular dynamics simulations of the pullout of a CNT from a cured epoxy resin. The simulations will be performed for both single wall nanotubes (SWNT) and multiwall nanotubes (MWNT). Based on the simulations, the interfacial shear strength between the nanotube and the cured epoxy resin will be calculated. Furthermore, it will be investigated whether there is an effective stress transfer from the epoxy resin to the nanotube. The simulations, preferably, will be performed with open source molecular modeling code LAMMPS and will be verified with the available results in literature.



Single wall carbon nanotube



Pullout of CNT from Polymer

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