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Evaluation of properties Carbon Nanotubes (CNTs) and CNT/polymer composites

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ABSTRACT

The mechanical properties of carbon nanotubes, such as high elastic modulus and tensile strength, make them the most ideal and promising reinforcements in substantially enhancing the mechanical properties of resulting polymer/carbon nanotube composites. It is acknowledged that the mechanical properties of the composites are significantly influenced by interfacial interactions between nanotubes and polymer matrices. The current challenge of the application of nanotubes in the composites is hence to determine the mechanical properties of the interfacial region, which is critical for improving and manufacturing the nanocomposites. In this work, a new method for evaluating the elastic properties of the interfacial region is developed by examining the fracture behavior of carbon nanotube reinforced poly (methyl methacrylate) (PMMA) matrix composites under tension using molecular dynamics simulations. The effects of the aspect ratio of carbon nanotube reinforcements on the elastic properties, i.e. Young's modulus and yield strength, of the interfacial region and the nanotube/polymer composites are investigated. The feasibility of a three-phase micromechanical model in predicting the elastic properties of the nanocomposites is also developed based on the understanding of the interfacial region.

Key words: Carbon Nanotubes, Mechanical Properties, Polymer, Composits, Elastic Properties.

1.INTRODUCTION

Since the documented discovery of carbon nanotubes (CNTs) in 1991 by Iijima and the realization of their unique physical properties, including mechanical, thermal, and electrical, many investigators have endeavored to fabricate advanced CNT composite materials that exhibit one or more of these properties. For example, as conductive filler in polymers, CNTs are quite effective compared to traditional carbon black microparticles, primarily due to their large aspect ratios. The electrical percolation threshold was recently reported at 0.0025 wt.% CNTs and conductivity at 2 S/m at 1.0wt.% CNTs in epoxy matrices. Similarly, CNTs possess one of the highest thermal conductivities known, which suggests their use in composites for thermal management. The main focus of this paper, however, will be on the use of CNTs as discontinuous reinforcement for polymer matrices. The CNT can be thought of as the ultimate carbon fiber with break strengths reported as high as 200 GPa, and elastic moduli in the 1 TPa range. This, coupled with approximately 500 times more surface area per gram (based on equivalent volume fraction of typical carbon fiber) and aspect ratios of around 103, has spurred a great deal of interest in using CNTs as a reinforcing phase for polymer matrices [1,2].

The outstanding electrical, mechanical, and thermal properties of carbon nanotubes (CNTs) have made them among the most promising materials in a wide range of applications such as nano-sensors and atomic transportation. In addition, the excellent mechanical properties of CNTs, such as ultra-high Young's modulus around 1 TPa and tensile strengths varying from 11–63 GPa, are promising ultra-high-strength reinforcements in high-performance polymer matrix composites.

2.Structure of Nanotubes

The primary symmetry classification of a CNT divides them into achiral or chiral [1]. An achiral nanotube is defined by a nanotube whose mirror image has an indistinguishable structure to the original one. And, as a