

## Chapter 19

# A Molecular Dynamics Simulation Study of the Mechanical Properties of Carbon–Nanotube Reinforced Polystyrene Composite

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### ABSTRACT

*In recent years, polymer/carbon nanotube composites have attracted increased attention because the polymer properties have significantly improved. In this paper, a single walled carbon nanotube (SWCNT) is used to reinforce polystyrene matrix. Molecular dynamics (MD) simulations are used to study two periodic systems - a long CNT-reinforced polystyrene composite and amorphous polystyrene matrix itself. The axial and transverse elastic moduli of the amorphous polystyrene matrix and nanocomposites are evaluated using constant-strain energy minimization method. The results from MD simulations are compared with corresponding rule-of-mixture predictions. The simulation results show that CNTs significantly improve the stiffness of polystyrene/CNT composite, especially in the longitudinal direction of the nanotube. Polystyrene possesses a strong attractive interaction with the surface of the SWCNT and therefore play an important role in providing effective adhesion. The conventional rule-of-mixture predicts a smaller value than MD simulation where there are strong interfacial interactions. Here the authors report a study on the interfacial characteristics of a CNT-PS composite system through MD simulations and continuum mechanics.*

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## 1. INTRODUCTION

There has been intense interest in carbon nanotubes (CNTs) since their discovery by Iijima (1991), because they possess exceptional stiffness, extraordinary resilience, remarkable thermal and electrical properties which conceivably, could have a far reaching impact on the next generation of advanced products (Lau & Hui, 2002). Due to their excellent structural, mechanical and electrical properties, CNTs are considered as potential candidate for reinforcement of polymeric materials (Thostenson, Ren, & Chou, 2001). Carbon nanotubes occur as single walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) (Ash, Siegel, & Schadler, 2004). A SWCNT can be viewed as a single sheet of graphite (i.e. graphene), which has been rolled into the shape of a tube (Saito, Dresselhaus, & Dresselhaus, 1998). SWCNTs have radii on the order of nanometers and lengths on the order of micrometers resulting in large aspect ratios beneficial to their use in composites (Roche, 2000; Saito, Dresselhaus, & Dresselhaus, 1998). Many believe that CNTs may provide the ultimate reinforcing materials for the development of a new class of nanocomposites. However, improvements in properties are by no means guaranteed, and the results are often sensitive to the particular polymer chosen, in addition to the quantity and quality of CNTs used in the composite. If we attempt to trace what controls the performance of materials, we can identify that properties of materials are largely dictated by the atomic structure, composition, microstructure, defects and interfaces in materials (Schaffer et al., 1995). As a result, it is very important to quantitatively understand the mechanics and physics of nano-structured materials, and only then we can effectively employ them in multi-scale material design.

Experimental measurement of the effective properties of CNT reinforced polymer matrix composites have indicated substantial increases in

the composite modulus over the matrix modulus. Schadler, Giannaris, & Ajayan (1998) found a 40% increase in the effective stiffness of CNT reinforced epoxy as compared to the matrix value with 5% weight CNTs Qian et al. (2000) also found an increase in the effective modulus of CNT reinforced polystyrene to be of the order of 40% for just 1% weight CNTs. Similar results were also reported by Xu et al. (2002) for MWNT/epoxy resin composites. A wide variety of composites containing CNTs have been manufactured. Peigney et al. (2000) have fabricated composites of CNTs embedded in ceramic powders while Milo, Shaffer, and Windle (1999) have embedded CNTs in poly vinyl alcohol.

The extent to which mechanical reinforcement can be achieved depends on several factors, including uniformity of dispersion, degree of alignment of CNTs, and the strength of polymer–CNT interfacial bonding (Han & Elliott, 2007). Since it is difficult to control and measure many of these properties experimentally, computational modeling can provide some crucial insights. For this reason, theoretical and computational methods have been widely applied to study polymer/CNT composites. In particular, molecular dynamics (MD) simulation can provide the ultimate detail concerning individual particle motions as a function of time. Thus, it can be used to address specific questions about the properties of a model system, often more easily than experiments on the actual system. Of course, experiments play an essential role in validating the simulation methodology, comparisons of simulation and experimental data serve to test the accuracy of the calculated results and to provide criteria for improving the methodology. In several earlier works, MD simulations have been successfully applied to the predictions of elastic properties of polymer-CNT composites. Frankland et al. (2003) used MD simulations to generate the stress-strain behaviour of polyethylene-carbon nanotube (NT) composites mechanically loaded in both the longitudinal and

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