C. R. Mecanique 343 (2015) 371–396

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

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Thermo-mechanical characterization of multi-walled carbon nanotube reinforced polycarbonate composites: A molecular dynamics approach

Sumit Sharma [a,*,1], Rakesh Chandra [b,2], Pramod Kumar [b,3], Navin Kumar [c,2]

[a] *School of Mechanical Engineering, Lovely Professional University, Phagwara, India*
[b] *Department of Mechanical Engineering, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar, India*
[c] *School of Mechanical, Materials & Energy Engineering (SMMEE), Indian Institute of Technology, Ropar, India*

ARTICLE INFO

Article history:
Received 31 January 2015
Accepted 11 March 2015
Available online 23 April 2015

Keywords:
Carbon nanotube
Damping
Mechanical properties
Molecular dynamics
Polycarbonate
Thermal conductivity

ABSTRACT

The present study aims at examining the mechanical properties of multi-walled carbon nanotubes–polycarbonate composites (MWCNT–PC), through a molecular dynamics (MD) simulation. Composites of MWCNT–PC were modeled using Materials Studio 5.5 software. Multiwall carbon nanotubes (MWCNTs) compositions in polycarbonate (PC) were varied by weight from 0.5% to 10% and also by volume from 2% to 16%. Forcite module in Materials Studio was used for finding mechanical properties. A marked increase in the elastic modulus (up to 89%) has been observed, even with the addition of a small quantity (up to 2 weight %) of MWCNTs. Also, upon addition of about 2 volume % of MWCNTs, the elastic modulus increases by almost 10%. The increase in mechanical properties is found to supplement earlier experimental investigations of these composites using nano-indentation techniques. Better load transfer property of MWCNTs, larger surface area and interaction between reinforcement with base matrix are the suggested reasons for this increase in mechanical properties.

1. Introduction

Carbon nanotubes are excellent reinforcements for polymers because of their unique mechanical properties and large surface area per unit volume. Experiments and calculations show that nanotubes have a modulus equal to or greater than the best graphite fibers, and strengths at least an order of magnitude higher than typical graphite fibers. For example, the measurement of the tensile properties of individual multi-walled carbon nanotubes (MWCNTs) gave values of 11–63 GPa for the tensile strength and 270–950 GPa for Young's modulus, as obtained by Yu et al. [1]. For comparison, the modulus and strength of graphite fibers are 300–800 and 5 GPa, respectively. In addition to their outstanding mechanical properties, the surface area per unit volume of nanotubes is much larger than that of embedded graphite fibers. For example, 30-nm-diameter nanotubes have 150 times more surface area than 5-μm-diameter fibers for the same filler volume fraction, such that the nanotube/matrix interfacial area is much larger than that in traditional fiber-reinforced composites. The

* Corresponding author. Tel.: +91 8146871758.
E-mail address: sumit_sharma1772@yahoo.com (S. Sharma).

[1] Assistant Professor.
[2] Professor.
[3] Associate Professor.

http://dx.doi.org/10.1016/j.crme.2015.03.002

unusual mechanical strength of the carbon nanotubes has motivated scientists to fabricate and modify other useful materials which are cheaply available in bulk form, by combining them as composites with carbon nanotubes. Polycarbonate (PC) is a lightweight polymer that is available in bulk form and is widely used for several engineering applications due to its moldability. For taking advantage of the useful properties of polymers in combination with unique structural properties of carbon nanotubes, multi-walled carbon nanotubes–polymer composites have been researched and fabricated over the past few years. In order to exploit the usefulness of these composites for specific mechanical engineering applications, their static and dynamic mechanical properties need to be evaluated. Among the static properties, the elastic modulus of the specimen is very important.

A lot of work has been published related to tensile testing of MWCNT–PC composites. These tests have evidenced that minor compositions (up to 2 wt. %) of MWCNT in PC enhance the modulus and tensile strength from 10% to even 70%. Choi et al. [2] used styrene and acrylo-nitrile (SAN) grafted MWCNTs with PC instead of pristine MWCNTs and observed that when SAN-grafted MWCNTs (1 wt. %) were used with PC, both tensile strength and modulus increased by nearly 5% and 10%, respectively, in comparison to pristine MWCNT–PC composites. Liu et al. [3] observed that at 3 wt. % MWCNTs in a PC, the composites exhibited a nearly 40% higher tensile strength in comparison to pure PC. However, for a 5 wt. % MWCNT composition, the strength reduced drastically. There are also contrary results obtained by Olek et al. [4], who reported no improvement in the presence of MWCNTs in the polymer poly-methyl-methacrylate (PMMA) for any static mechanical property. Even with a compositional change from 1% to 5% of MWCNTs, the elastic modulus remained almost the same as that of pure PMMA. However, if the MWCNTs were coated with silica, the composite showed remarkable results upon nano-indentation. With only 4% MWCNT–silica in PMMA, the modulus measured is about three times that of pure PMMA. Reinforcement on poly-vinyl alcohol (PVA) and PMMA with few-layer graphene (FG) was also tested using a nano-indenter by Das et al. [5].

Low compositions of FG (0.6%) in PVA made the modulus increase by about 20%. Vivekchand et al. [6] have explained the use of inorganic nanowires (NW) as reinforcement in PVA to be as efficient as MWCNTs. The elastic modulus increased by almost two times upon reinforcement by 0.8% (in volume) of inorganic NW. However, MWCNTs have a very smooth surface; making the strength imparted by reinforcing with MWCNTs lesser than with NW. Kim et al. [7] used a compatibilizer as two poly-g-polycapro-lactones (P3HT-g-PCLs) with bisphenol-A-PC-MWCNT composite. When a PC-MWCNT composite was combined with P3HT-g-PCL, then there was an increase of nearly 22% in the Young modulus and 30% in the tensile strength in comparison to pure PC. For small concentrations (0.1–0.5 wt. %) of MWCNTs, this increase was found to be consistent. However, when the MWCNTs concentration was further increased to 1 wt. %, then both Young's modulus and tensile strength were considerably reduced.

Eitan et al. [8] used bisphenol-A-PC with MWCNTs as composites for mechanical characterization. Tensile tests were performed using a Universal Testing Machine and it was found that for composites with surface-modified MWCNTs (5 wt. %), the modulus improved by 95% in comparison to pure PC. Even for composites using pristine MWCNTs (5 wt. %), the modulus rise was nearly 70% in comparison to pure PC. Ayatollahi et al. [9] have used epoxy-MWCNT composite under shear and bending load using a Santan Universal Testing Machine. They have also found that there is a gradual increase in elastic modulus and tensile strength as MWCNT composition increased in epoxy. Compositions of 0.1%, 0.5% and 1.0% MWCNTs in epoxy were fabricated and, as the composition of MWCNTs increased, both elastic modulus and tensile strength increased by 10%. Montazeri et al. [10] used a Hounsfield machine and also evaluated the viscoelastic behavior of epoxy-MWCNT composite. They reported that with further increase in MWCNT composition of 2%, the elastic modulus increased by about 20% as compared to pure epoxy samples.

Computational studies complement experiment by providing easy manipulation, analysis and insights into the molecular level. 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. 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.

Due to the difficulties in the experimental characterization of nanotubes, computer simulation has been regarded as a powerful tool for modeling the properties of nanotubes. Among the available modeling techniques, molecular dynamics simulation has been used most extensively. First-principles methods are able to generate reasonably accurate data of structures and energies relevant to polymer nanocomposite systems, but they can only be used to study small systems over short times due to their computational expense. In contrast, molecular simulation methods such as molecular mechanics (MM) and molecular dynamics (MD), which are based on analytic force fields, are computationally cheaper compared to first-principles methods. They can therefore be used to study larger molecular systems for longer times. As described below, MD can also be used to obtain macroscopic properties such as the Young modulus.

The present study was undertaken to investigate changes in the static mechanical properties under the influence of varying compositions (per weight and per volume) of pristine MWCNTs in PC by employing the MD technique without any additional component or any surface modification in the composite. The elastic modulus has been studied to supplement the experimental investigations on these composites made by Kumar et al. [11]. They prepared composites of MWCNT–PC by a two-step method of solution blending, followed by compression molding. Multiwall carbon nanotubes (MWCNTs) compositions in polycarbonate (PC) were varied by weight from 0.5% to 10%. Nano-indentation techniques were used to evaluate mechanical properties like elastic modulus and hardness. A marked increase in the elastic modulus (up to 95%) was observed with the addition of small quantities (up to 2 wt. %) of MWCNTs.