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Investigation of the structural and mechanical properties of polypropylene-based carbon fiber nanocomposites by experimental measurement and molecular dynamics simulation

Shin-Pon Ju [a,b,*], Chien-Chia Chen [a], Tien-Jung Huang [c,d,*], Chun-Hsiung Liao [c], Hsin-Lung Chen [d], Ying-Chen Chuang [a], Yng-Ching Wu [a], Hsin-Tsung Chen [e]

[a] Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-Sen University, Kaohsiung 804, Taiwan
[b] Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 807, Taiwan
[c] Material & Chemical Research Laboratories, Industrial Technology Research Institute, Hsinchu 310, Taiwan
[d] Department of Chemical Engineering, National Tsing Hua University, Hsinchu 300, Taiwan
[e] Department of Chemistry, Chung Yuan Christian University, Chung-Li 320, Taiwan

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ABSTRACT

This study investigates the interfacial strengths between polypropylene (PP)/carbon fiber (CF) composites through experimental observation as well as using molecular dynamics (MD) simulation to determine optimal chemical functionalization groups for four PP/CF composites. First, the structures of PP/CF, PP-*graft*-maleic anhydride (PP-MAH)/CF, PP-MAH/CF-NH_2 (2%) and PP-MAH/CF-NH_2 (5%) were constructed to obtain stable interface structures by the simulated-annealing procedure, and these structures were further used to evaluate the interface bonding strength. The study found that the degrees of crystallinity of PP and PP-MAH at the interfaces are significantly improved when compared to those of the pristine structure. The results show, through the interaction energy per unit area and the tensile simulation mechanical strength, that the strengths of the modified PP/functionalized-CF are higher. Finally, the MD simulation results of the modified PP and functionalized-CF composites are demonstrated to provide an economical and quick approach to examine the mechanical properties of a polymer composite system before conducting an experiment. Such MD results can be utilized to guide both the design of polymer/carbon fiber composites and to select proper functionalized groups.

1. Introduction

Recently, polymeric nanocomposites have played a significant role in the development of nanomaterial fabrication because these polymeric nanocomposites provide value-added properties as compared to pristine polymer without sacrificing its material properties. These include inherent mechanical properties and lighter weight as well as increased processibility. Polypropylene (PP) is a polyolefin polymer used in a wide variety of applications. PP has been used as the matrix material in a commercial form because of its many attractive properties, such as low weight, relatively low cost, excellent heat distortion temperature (above 100 °C) and its recycling ability [1]. Accordingly, PP was used in this study as the polymer matrix of a composite material in order to investigate its mechanical properties.

There are two main ways to improve the mechanical properties of polymer materials: the first is to alter the crystalline interfacial regions the polymer material [2,3], resulting in better stress transfer, and the second is to mix the polymer with certain fillers in order to form a polymer composite material [4]. The former is not suitable for most polymers because their conformations of structure are inherently amorphous [5]. The latter method, therefore, is more promising for the current study because polymer composites demonstrate excellent thermal, mechanical, and electrical properties [6–8]. One of the most popular composite materials is a combination of carbon fiber (CF) and polymer.

Among carbon related materials, CF is a popular reinforcement material due to its high stiffness, high tensile strength, excellent creep resistance and light weight. As such, it is a good candidate

* Corresponding authors at: Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-Sen University, Kaohsiung, Taiwan. Tel.: +886 7 5252000 4231; fax: +886 7 5254299 (S.-P. Ju). Material & Chemical Research Laboratories, Industrial Technology Research Institute, Hsinchu, Taiwan. Tel.: +886 3 5915330; fax: +886 3 5830239 (T.-J. Huang).

E-mail addresses: jushin-pon@mail.nsysu.edu.tw (S.-P. Ju), tjhuang@itri.org.tw (T.-J. Huang).

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to act as a filler material that enhances the mechanical properties of polymer materials. In addition, CF is relatively cheap when compared to carbon nanotubes. Currently, it can be produced in high volumes at low cost, another advantage of using it as a filler for mechanical property enhancement [8].

The production process of CF and polymer composites is relatively simple and inexpensive. One of the most important factors in the design of the composite is the interface quality between CF and polymer matrix [9,10]. In recent years, many researchers have investigated the chemical reaction between the CF and polymer. If hydrogen bonds form between the modified CFs (hydrophilic), the CFs then distribute homogeneously throughout the non-polar polymer matrix at the microscopic level [9]. This improves the interfacial adhesion and provides a larger area during load transference by increasing the chemical interaction between the CF surface and the polymer matrix [10]. The excellent fracture behavior of polymer composites is also dependent on the high strength of its interface [11]. In order to improve the chemical interaction of the CF surface with the polymer matrix, a variety of surface treatments have been developed, such as the application of coupling agents, oxidation, and grafting [12–14], all of which introduce chemically active groups to increase the interfacial bonding between the polymer matrix and the CF [15]. The studies above have demonstrated that interfacial adhesion has a significant effect on the mechanical properties of composite materials, and this interfacial adhesion can be affected by grafting a functional group component. Hence, the interfacial strength between the CF/PP composite is here investigated by grafting a functional group.

Since direct investigation of the interfacial characteristics of polymer composites by experiment is somewhat difficult due to the very small scales involved, numerical methods such as molecular dynamics (MD) are generally preferred. Adopting this technique, Lv's study [16] use MD simulation to look at how chemical functionalization of graphene affects the interfacial bonding between functionalized graphene and polymers. Their results show that bonding energy and shear stress at the graphene/polymer interface increases with increased concentrations of the functionalized group. In Zhang's study [17], MD simulations were used to examine hydroxyapatite/biopolymer interface interactions in composites used primarily in biomedical applications. The study analyzed the binding energies between hydroxyapatite (HA) and three polymers: polyethylene (PE), polyamide (PA) and polylactic acid (PLA), with results showing that PA/HA and PLA/HA binding energies are much higher than that of PE/HA. Zhang et al. suggested that this might be due to the large number of polar groups in the PA and PLA chains. In these papers, MD simulation was proven to be a proper simulation technique useful for studies of the interfacial characteristics of polymer composites.

The properties of the CF/polymer interface significantly influences the mechanical behaviors, but is very difficult to investigate empirically. In this study, the experimental approach was used to determine the mechanical properties of PP/CF as well as PP-*graft*-maleic anhydride (PP-MAH)/CF, which were constructed using the hot press method. The surface topography of the composites as well as the distribution of PP sheets in the interfacial region of CFs was also examined by scanning electron microscopy (SEM). In addition, MD simulation was performed to investigate the structural variations between PP/CF and modified PP-MAH/CF interfaces under a tensile load. We also used MD to examine the microstructures with the aim of explaining the polymer matrix/CF interfacial properties. Finally, a prediction of the interfacial properties of the PP/CF composite with different functional groups was conducted using the PP/graphene model to determine the preferred interfacial properties of the composite.

2. Materials and methods

2.1. Experimental detail

This study investigates the mechanical properties of a composite system composed of a polypropylene (PP) polar modification polymer material and CF. Modified PP pellets (trade name Fusabond P613) were obtained from E.I. du Pont de Nemours Company, maleic anhydride was obtained from Echo Chemical Co., Ltd., and CFs (Toho Tenax HTS40) were purchased from Sakai Ovex Co., Ltd. The small amounts of NH_2 in the functionalized CF, as well as the amount of MAH in the modified PP, were both kept at 1%. Samples, dimensions of length = 20 cm and width = 20 cm, were prepared by using hot press forming, a thermal bonding procedure. The comparison sample (notated as PP/CF), which mixes the PP and CF, both without polar modification, has a CF content of about 56.1 wt%. The experimental sample (notated as PP-MAH/CF-NH_2), which mixes the PP and CF with polar modifications (i.e., with MAH and NH_2 functionalized groups), has a CF content of about 57.8 wt%. The adhesiveness of the CF and the PP were observed by using a scanning electron microscope (SEM). The difference in adhesiveness between the experiment and comparison samples is studied and their simulated mechanical strengths are compared to better understand factors affecting mechanical properties and improve modification of material.

2.1.1. Hot press forming

The hot press machine used for hot press forming is a DAKE 44-350. The temperature of the warm-up process was 260 °C. The hot press sheets were prepared using PP both with and without polar modification, and were placed into a baking machine to be dried. The dried hot press sheets were preheated to 260 °C for 10 min, and pressurized at 200 psi for 2 min at 260 °C. Then the plate was placed on the bottom portion of the hot-pressing device and cooled at 200 psi with cool water for 5 min. Finally, the hot-pressed specimens were removed, and their thicknesses were measured by a Vernier caliper. A total of 12 of each specimen were produced.

2.1.2. Thermal bonding forming

In order to prepare a sample thick enough for mechanical testing, the sheets of the PP both with and without polar modification were sandwiched with the CF and laminated. The thickness of the CF cloth and PP sheets are 0.2 and 0.1 mm, respectively. As shown in Fig. 1, a laminated structure consisting of 6 alternating layers (3 each) of PP sheet and CF cloth is then formed by thermal bonding, with a 5 min warm-up process at 260 °C, and pressurizing for 2 min at 800–900 psi. Next, the laminated material was moved to another pressing device and was cooled at 1200 psi for 2 min. The sample size is 0.6 mm thick after thermal bonding formation.

2.1.3. Mechanical properties testing

An Instron 1186 at a load of 1000 kg was used for the tensile strength test. The tensile strength test was performed according

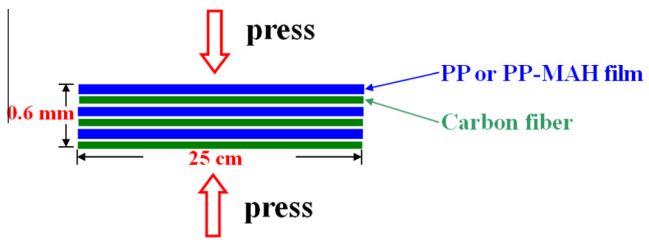

Fig. 1. Schematic illustration of experimental sample preparation.