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Reinforced thermoplastic composites with interfacial microarchitectural anchoring: Computational study

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ABSTRACT

Reinforcing potential of fibers is limited for a number of thermoplastic polymers due to the inherently weak interfacial bonding between the non-polar/non-reactive polymer matrix and fiber surface. To this end, the concept of enhancing the interfacial strength in thermoplastic composites via controlled mechanical interlocking between fiber surface and polymer matrix is explored. Specifically, infiltration of the thermoplastic polymer into the anchoring sites around the microstructures located on the fiber surface provided an efficient mechanical interlocking. A computational study has been performed for several different surface morphologies for a glass/polyethylene material system. The strength calculations addressed both material failure and detachment of the matrix material from the anchoring sites. The results obtained, which focused on shear loading, indicated that the surface morphology has a significant effect on the interfacial bonding strength. The computational analysis results showed that even without any interfacial friction or adhesion, the interface strength could achieve 50% of the theoretical strength of perfect matrix-fiber bonding for a plane interface. An optimal geometry and density of the microarchitectured features on the surface was identified for many cases in a parametric study. Friction at the interface between polymer matrix and fiber surface was shown to provide a significant increase in interfacial strength for cases where the frictionless case detached, but not for cases of material failure, which shows the promise of anchoring when friction and adhesion cannot be relied on. It was therefore demonstrated that the precise surface morphology modification is an effective approach to improve the interfacial bonding in fiber reinforced thermoplastic composites.

1. Introduction

The overwhelming majority (~ 90%) of modern polymer materials are thermoplastics that are melt processed in an industrial setting (Fried, 2003; American Chemistry Council, 2016; Ehrenstein, 2001). Compared to thermosets, thermoplastic polymers have several significant advantages (Fried, 2003; Ehrenstein, 2001). Thermoplastic polymers can be formed quickly into complex geometries due to their low viscosity at high temperature. They can be easily reproduced and have extended shelf life. The manufacturing cost is typically low and the materials can be readily recycled. Other benefits include improved chemical resistance, increased mechanical toughness, high ductility, and, for a number of thermoplastics, high glass-transition/melting temperature. For these reasons thermoplastic polymer composites are increasingly replacing thermoset composites in many applications, as they offer sustainable lightweight solutions that combine the high strength of a metal with the corrosion resistance of a plastic.

From the commercially available thermoplastics approximately 60% are either polypropylene (PP) or polyethylene (PE) (American Chemistry Council, 2016). While thermoplastic polyolefin composites have many advantages, poor adhesion between thermoplastic polymer matrix and high stiffness/strength reinforcement fillers such as carbon and glass fibers, has hindered their use in automotive, aerospace, defense and consumer product applications (Tiwari and Bijwe, 2014). In fact, both PP and PE have low surface energy (van Krevelen, 2000) and it is difficult to obtain a chemical reaction between the thermoplastic and carbon fiber functional groups (Varelidis et al., 1999). These materials form only weak van der Waals bonds with the fiber surface and, therefore, demonstrate low interfacial adhesion. For example, the bond strength is typically less than 1 MPa for thermoplastic polymer matrix composites containing ceramic fillers with no surface treatment (Li et al., 1994).

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To overcome this challenge, various approaches have been proposed to enhance the adhesion of thermoplastic polymers to fiber surfaces. The interface strengthening mechanisms can be broadly categorized into physical and chemical modification methods. Physical modification methods can be further categorized into macroscopic modification approaches such as fiber fibrillation (Li et al., 1994) and polymer rivet (Grujicic et al., 2008), and microscopic methods including sputter etching to increase surface roughness (George et al., 2001), plasma treatment (Liu et al., 2014), and grit blasting with micro particles for mechanical interlocking (Grujicic et al., 2008; Schulze et al., 2013). Chemical modification methods include grafting (George et al., 2001; Etcheverry and Barbosa, 2012; Peng et al., 2013) to form covalent bonds, and coating coupling agent layers such as silane (George et al., 2001; DiBenedetto, 2001; Cho et al., 2004), isocyanate, or titanate compounds (George et al., 2001), electrochemical treatment (Liu et al., 2012b; Vautard et al., 2013) and oxidation (Guo et al., 2009; Li, 2008). Among these strengthening mechanisms, macroscopic physical modification cannot be applied to fiber-reinforced thermoplastics due to the microscopic length scale of the fibers. Existing microscopic physical modifications such as sputter etching and grit blasting lack control of the microscopic features imprinted on the surface, which is believed to be an essential element of the microarchitectural anchoring studied herein. An effective technique that produces a significant number of covalent bonds between polymer matrix and fiber and, therefore, higher interface strength is polymer covalent grafting (George et al., 2001; Etcheverry and Barbosa, 2012). For example, interface strengths of 6 MPa have been reported for PP grafted from the surface of glass fibers by surface initiated polymerization (Etcheverry and Barbosa, 2012). While this level of increase is impressive, it comes at a very high cost. Another more economical way to improve the thermoplastic/glass fiber interface is to add a polymer modified with reactive groups capable of forming covalent bonds with the fiber surface. For PP and PE this is typically achieved by adding 1–10% of maleic anhydride (MA) monomeric units to the polyolefin macromolecules as a short side chain (Chung, 2002; Rijsdijk et al., 1993; van den Oever and Peijs, 1998; Yuan et al., 2011). However, only incremental improvements of the mechanical properties of the polymer modified with MA have been reported for glass fiber composites (Rijsdijk et al., 1993; van den Oever and Peijs, 1998). This result indicates that only a small fraction of the reactive MA units can reach the fiber surface for the reaction and most of the surface contacts are weak van der Waals bonds. Transcrystallinity tailoring of the interface for PP/glass fiber or carbon fiber composites is also shown to enhance interfacial strength. The measured strength using pull out tests can be as high as 5–10 MPa (Wang and Chen, 1999; Wu et al., 2001; Li et al., 2013).

Fiber sizing is another commonly used technique that improves interfacial bonding strength in fiber reinforced plastics. The fiber surface is often coated with nanoparticles or a polymer layer to increase the surface roughness and provide mechanical interlocking (Liu et al., 2012a; Wu et al., 2016; Qin et al., 2015; Gao et al., 2011; Dey et al., 2014; Jiang et al., 2015). In the recent studies, carbon nanotubes (CNTs) were also used as a modification to fiber surface to enhance the composite properties (Siddiqui et al., 2011; Sun et al., 2016; An et al., 2012). Apparently, sizing and CNT treatment of fibers provide enhanced bonding between fiber and matrix through the mechanism of mechanical interlocking with an increase in surface roughness. The main focus of the present study is that a precise and controlled modification of the fiber surface could provide an even better bond.

In this paper, a novel concept to enhance interfacial strength of thermoplastic composites with non-metallic reinforcements is proposed. This is achieved via controlled mechanical interlocking through precise surface topology modification to create a microarchitectured arrangement of sites to transfer load at levels much higher than with the other approaches. Surface topology modification can be performed on either one of the material phases at the interface. For example, in a recent study nanoimprint lithography was used to modify polymer substrate surface for evaporation deposition of metal thin film for flexible electronics applications (Eom et al., 2015). For thermoplastic composites, on the other hand, we propose to modify the surface of the reinforcement phase with various microarchitectural features. For instance, beads, voids, cavities, etc. could be realized experimentally for different reinforcement materials. Examples include thin carbon films with controlled pores on the surface (Peng et al., 2016; Ozsoy et al., 2015) and single or multilayered assemblies of nanoparticles on glass surfaces (Malynych et al., 2002; Kokuoz et al., 2009). The techniques used to create the micro-structures on the carbon and glass films are applicable to fiber surfaces as well.

Computational analyses are performed systematically for several different surface morphologies for a glass/polyethylene material system. Specifically, the stresses and failure modes at the glass/polymer interface are studied in detail. The dependence of the interfacial strength on the morphology and geometric parameters of the surface microarchitecture is elucidated through parametric studies. The results show that microarchitectural anchoring with precise control could be a cost effective way to achieve significant improvement, and hence alleviate to a significant extent the problem of weak interfacial adhesion in these material systems.

The remainder of the paper is organized as follows. Section 2 presents the finite element model for the mechanical analysis of the interfacial microarchitectural anchoring. This section also includes the material model and failure modes. Section 3 presents the results and discussions. Conclusions follow in Section 4.

2. Finite element modeling of mechanical interlocking strength

2.1. Approach

Since the purpose of this study is to understand how the surface microarchitectural features affect the interfacial bonding strength between two materials (thermoplastic polymers and reinforcement materials such as glass and carbon), without loss of generality, we focus on an idealized model composite system, that can easily be fabricated, where the thermoplastic polymer matrix is reinforced by glass layers with rod-like microarchitectural features, as shown in Fig. 1a.

Experimentally, the push-out test has been commonly used to investigate bonding strength between fibers and matrix (Zhandarov and Mader, 2005; You et al., 2009). In the push-out test the fiber is pushed in the axial direction with an indenter. Displacement of the indenter is measured as the load is increased. The resulting force-displacement curve can be used to estimate when interface fracture initiates and progresses by observing decreases in load. In a similar manner, a hypothetical shear test is performed computationally herein by using the finite element analysis package ABAQUS on a three-layer composite made of a glass layer sandwiched by two layers of polymer (Fig. 1a) to assess the glass/thermoplastic interfacial bonding strength. As shown in Fig. 1a and b, the shear test is performed under conditions of plane strain by applying a vertical displacement to the glass layer.

2.2. Computational domain

As illustrated in Fig. 1b, symmetry can be used to model half of the test specimen. Further utilizing the periodicity in the geometry (Fig. 1b) and deformation (Fig. 1c), a unit cell or representative volume element (RVE) with periodic boundary conditions

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