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Micromechanics of diffusion-induced damage evolution in reinforced polymers

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ABSTRACT

In this work we numerically investigate the nucleation and evolution of micromechanical damage in reinforced glassy polymers under transient hygro-mechanical loading. In particular, we demonstrate the role that fiber distribution plays in the evolution of overall damage due to fiber–matrix interfacial debonding under moisture ingress. The heterogeneity of fiber distribution (clustering) is characterized by the coefficient of variation C_v of the center-to-center distances between interacting fibers, determined by identifying a cut-off radius around a typical fiber. The initial moisture diffusion-induced damage provides synergistic conditions for the rapid evolution of debonding under subsequent mechanical loading. The results indicate that microstructural heterogeneity strongly affects the moisture diffusion characteristics that in turn hurt the overall load carrying capacity of a composite due to aggravated damage. The strong dependence of the moisture-induced damage evolution on the fiber arrangement suggests that one should not resort to using simplistic unit cell models that assume regular fiber arrangements in such cases.

1. Introduction

Polymers, natural or synthetic, are often reinforced with stiffer inclusions in the form of fibers or particles to create heterogeneous composites that are attractive for applications where mechanical strength and stability are of primary interest. The choice of the polymer (matrix) and inclusion (reinforcement) is dictated by the requirements of the end application. Many large-scale structural applications such as automotive, aerospace, turbine blades, etc. typically employ epoxy-based polymeric matrices reinforced with high strength synthetic fibers such as glass or carbon. Often, the differences in the physical, mechanical and chemical properties of these two constituents create a large property mismatch in the interfacial regions of the composite. Under external stimuli, high stresses tend to concentrate around these interfacial regions and this may potentially lead to overall composite degradation through a variety of microstructural instabilities including interface debonding, fiber breaking, void nucleation and shear localization in the matrix that are precursors to the macro-structural failure. It has long been recognized that while polymer composites possess exceptional potential in designing light and strong applications, their use may be limited by the fact that their response to environmental conditions during their functional life is not well understood. This is especially critical when one recognizes that they are deployed in protean service environments and are expected to perform over long periods of time. Residual stresses occur in a composite subjected to varying temperature or moisture conditions, due to the difference in the thermal or moisture expansion coefficients between the fiber and the matrix. In particular, moisture ingress may assist the degradation of composites, possibly further amplified by temperature, that may be detrimental, for example, wind energy or marine structures that experience a range of changes in temperature and moisture (salinity may have additional effects) in addition to the regular mechanical loads [1,2]. Composites used for dental restoration purposes may experience aqueous service environments that range between strongly acidic to strongly alkaline [3]. Further, the moisture diffusivity itself may be a function of the applied stress, which in turn may affect the stress distribution in the composite [4–6]. The absorbed moisture may lead to matrix cracking [7–11] or plasticize the matrix thereby reducing effective stiffness and strength of polymers [7] and their composites [1,2,12]. An efficient design of a composite for specific functions relies heavily on the ability to predict the possible mechanisms of failure at multiple length and time-scales when subjected to such synergistic environments [13,14]. These effects may be further complicated by the fact the most composite micro-architectures exhibit random inclusion topologies. The aforementioned scenarios pose challenges for engineers and necessitate a better understanding of the mechanical behavior of such heterogeneous micro-architectures in hostile environments as a function of microstructural details.

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In this work, we numerically investigate the response of reinforced glassy polymers under transient hygro-mechanical conditions at the microstructural length-scale. We focus on modeling the nucleation and evolution of damage at the micromechanical scale in a model glass-reinforced epoxy polymer composite subjected to moisture and mechanical loads under isothermal conditions. Of the above-mentioned possible microstructural modes of failure, we explicitly model the experimentally observed debonding at the matrix-inclusion interfaces due to moisture-induced stresses [2,15,16]. Such debonded interfaces may act as the channels causing accelerated diffusion especially if it is in the exposed surface [17]. Further, some experiments on glass fiber–epoxy matrix composites have revealed that both the strength and toughness of the fiber–matrix interfaces may degrade significantly in moist environments exacerbating the severity of damage [2,18]. Motivated by these experimental observations (see also [19]), we incorporate the possibility of the interface behavior that continuously degrades with the evolution of local moisture concentration. While the moisture diffusion and stress build-up phenomena in composites have been modeled by researchers (e.g. [20,21]), there are relatively few works that model the evolution of hygro-mechanically induced damage, in general (e.g. [6,22]) and interface failure, in particular (e.g. [23]). Some works that do model interfacial effects under hygral or thermal excursions resort to the restrictive assumption of unit cells with regularly arranged fibers (e.g. [24]), which is seldom the case in real materials [25]. In fact, the effective diffusivities may strongly be affected by the tortuosity of the microstructure, which may have direct implications on the build-up of differential stresses [21,25,26]. In this work, we relax this restriction by choosing representative volume elements (RVEs) with random arrangements alongside the regularly arranged RVEs. In précis, the objective of this work is to develop a predictive approach to characterize moisture diffusion-induced damage incurred through interfacial failure in reinforced polymers as a function of microstructural randomness and its effect on the subsequent response when loaded mechanically. In the next section, we describe the computational setup and the details of the finite element (FE) models used in the investigation.

2. Computational modeling

Fig. 1 shows a typical section of a unidirectionally reinforced lamina of thickness $2L_2 = 100$ μm [13] in the X_2-direction considered in the present work. We consider the lamina to be infinitely long in the X_1-direction, comprising repeating unit cells giving a periodic RVE in that direction (shown in the figure by the dashed box). Further, we assume that the lamina is symmetric about $X_2 = 0$ and satisfies the plane-strain condition in the X_3-direction. Within an RVE the fibers may be arranged in a regular or random manner. The top and bottom surfaces of the lamina may be subjected to mechanical and/ or moisture boundary conditions (bc's).

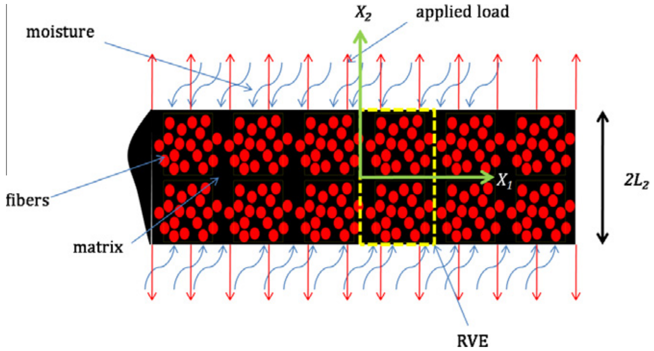

Fig. 1. A unidirectionally reinforced composite lamina subjected to mechanical and moisture boundary conditions. The lamina is periodic in the X_1-direction. A typical RVE considered in the computational modeling is shown by the dashed boundary.

2.1. RVE generation and characterization of micro-architectures

Microstructural characterizations of real composites unequivocally reveal the random topological arrangements of fibers (e.g. [27,28]). While one may use digitized versions of such real microstructures, we adopt a more computational approach in that we generate artificial microstructural arrangements mimicking real composites [29]. Such a strategy enables comparing a wide range of microstructures with different fiber volume fractions f, arrangements and fiber diameters, d. As an example, Fig. 2a–f shows six of the nearly 50[1] different RVEs considered in this work that are generated using an in-house code for two-dimensional (2D) heterogeneous composite micro-architectures with desired fiber arrangements (regular/random and uniform/clustered), for a given fiber diameter d and f. Specifically, these RVEs are constructed for fixed $f = 0.47$ for all the random arrangements and equal to 0.50 for the two regular arrangements to investigate the effects of fiber distribution. These volume fractions are represented by 15 (16 in the case of the regular arrangements) 10 μm diameter fibers [30], which also sets up the size of the RVE. The RVEs in Fig. 2a–c are three different random (R1, R2, R3) arrangements. Note that amongst these three the R2 arrangement has all the fibers completely inside the RVE, which means that there exists a thin *matrix-rich* layer at the edges of the RVE [25]. Fig. 2d shows a random arrangement but with a clustering (RC) of fibers leaving what appears to be a big region in the microstructure that is matrix-rich. Fig. 2e shows the regular square (SR) arrangement, used as benchmark. Finally, Fig. 2f shows the square clustered (SC) arrangement where a set of four fibers are placed close together and this arrangement is repeated within the RVE. This description of the RVEs with random fiber arrangements is qualitative. In literature, different approaches have been formulated to characterize the topological disorder in composite microstructures. Pyrz and Bochenek [31] defined topological entropy based on the Dirichlet tessellation method and correlated it with the microstructural stress field in fiber composites. Chen and Papathanasiou [28] used a second-order intensity function based on a cut-off radius and the number of fibers within that zone to characterize different fiber arrangements. Based on an exclusion probability defined by Torquato [32] few others [33,34] used the nearest neighbor distance. In this work, we quantify the heterogeneity of fiber distribution (i.e. clustering) in different RVEs using the center-to-center (c–c) distance between the neighboring fibers. The neighbors of a fiber are defined such that the lines joining the centers of two fibers do not trespass other fibers. Then, the coefficient of variation $C_v(=\Sigma/\mu$, Σ = standard deviation and μ = mean) of the c–c distance can be used as a metric to quantify clustering. Fig. 3 shows an example for the random arrangement with $d = 10$ μm and $f = 0.47$. Green circles are the fibers, the magenta outline represents the periodicity of the RVE, and the blue and red lines connect the centers of fibers such that none of the lines pass through an intermediate fiber. Note that the red lines connect fibers that are significantly apart from each other even though they may not necessarily *communicate* with each other through their stress fields, yet they can be connected topologically as far as the definition of c–c connectivity is concerned. From a topological perspective, this situation may not be uncommon in random microstructures; however, from the physical viewpoint it may not be relevant to include such remote influences. An important question then arises: for a given fiber, how many surrounding fibers influence its failure? In other words, is there a cut-off radius r_c that

[1] These include RVEs for different volume fractions (vf) (f = 0.30, 0.40, 0.50, 0.60) and diameters (d = 9, 10, 11 μm).