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Automated analysis of microstructural effects on the failure response of heterogeneous adhesives

Soheil Soghrati [a,b,c,*], Bowen Liang [a]

[a] Department of Mechanical and Aerospace Engineering, The Ohio State University, USA
[b] Department of Materials Science and Engineering, The Ohio State University, USA
[c] Simulation Innovation and Modeling Center (SIMCetenr), Columbus, OH, USA

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ABSTRACT

Adhesive bonding enables the joining of thin and dissimilar materials, which is one of the main requirements for manufacturing lightweight structures in the automotive and aerospace industries. However, due to the small thickness and complex microstructure of the adhesive layer, which is often reinforced with embedded heterogeneities to improve its mechanical behavior, simulating the damage process in the adhesive can be a challenging task. In this work, we implement a computational cohesive model to quantify the effects of microstructural features such as particles volume fraction, pre-existing flaws, and surface roughness of adherends on the failure response of a heterogeneous adhesive with embedded glass particles. The hierarchical interface-enriched finite element method (HIFEM) is implemented as the main computational engine for simulating the initiation and propagation of damage in the adhesive layer. This mesh-independent method allows for using finite element meshes that are completely independent of the problem morphology, which considerably facilitates conducting multiple damage simulations for adhesive models with different microstructural features. We also introduce a new virtual prototyping algorithm and integrate that with the HIFEM to enable the automated construction of realistic models of the adhesive microstructure based on digital data.

1. Introduction

Adhesive bonding offers several benefits over conventional methods of fastening, including a smooth exterior, sealing characteristics, reduced local stress concentrations (Hesebeck et al., 2007; Popelar and Liechti, 1997), higher shock absorption (Yang et al., 2012), better corrosion resistance (Sharland, 1987), and ease of joining thin and dissimilar materials. Due to such advantages, the application of adhesive joints is constantly growing in engineering structures and particularly within industries seeking light-weight solutions (Marques et al., 2015), such as the aerospace, automotive, and shipbuilding. Heterogeneities such as rubber, glass, and silica particles are often added to the polymeric adhesive matrix to improve its fracture toughness and provide multifunctionality (e.g., electrical conductivity) (Gojny et al., 2005; May et al., 2010). Thus, in addition to chemical considerations, determining optimal microstructural features such as the type, volume fraction, size, and morphology of embedded particles is crucial to the design of adhesives for improving structural performance.

Identifying the effect of heterogeneities on the mechanical behavior and damage toughness of adhesives has been the subject of several experimental studies(Korta et al., 2015; Markatos et al., 2013). To enumerate a few research works in this field, we can mention the study on the impact of silica particles size and volume fraction on the adhesive failure response (Imanaka et al., 2001; Hsieh et al., 2010); the characterization of the failure response of glass-filled adhesives with different surface treatments and moisture exposures (Kawaguchi and Pearson, 2003a, 2003b); and the study on the role of nano-Al_2O_3 particles on increasing the adhesion strength (Zhai et al., 2008). However, a limited number of studies have employed computational techniques such as the finite element method (FEM) to quantify the impact of adhesives heterostructure on their failure response, which can be attributed to two key challenges in simulating this problem: the small thickness of the adhesive layer and its complex microstructure.

The considerably smaller thickness of the adhesive layer (ranging from a few hundred microns to a few millimeters) compared to other characteristic length scales of structural components such as aircraft wings and automobile frames hinders the application of a direct numerical simulation (DNS) approach for performing failure simulations (Bogdanovich and Kizhakkethara, 1999). Thus, the concept of cohesive zone modeling (CZM) (Needleman, 1992;

* Corresponding author at: Department of Mechanical and Aerospace Engineering, The Ohio State University, USA. Tel.: +816142922768; fax: +816142922222.
E-mail address: soghrati.1@osu.edu, soheilsoghrati@gmail.com (S. Soghrati).

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De Borst, 2003; Spring and Paulino, 2014; Sørensen, 2002) has been introduced and widely implemented as a surrogate model for the analysis of adhesive-bonded structures. In this method, the adhesive layer is replaced with a lower-dimensional manifold with zero thickness (e.g., a surface in a 3D model), which is discretized using cohesive elements with a given traction-separation (cohesive) law to approximate the damage initiation and progression in this layer (Gustafson and Waas, 2009; Khoramishad et al., 2010; Reinoso et al., 2012).

While the CZM can significantly facilitate modeling structures with adhesive joints, the reliability of resulting simulations depends on the cohesive law adopted to describe the damage process in the adhesive layer (Alfano et al., 2015). Phenomenological models are among the most common cohesive models used in the CZM, which can be categorized as non-potential and potential based models (Park and Paulino, 2011). Although non-potential cohesive models are relatively easy to implement, one of their inherent shortcomings is the assumption of a constant fracture energy, regardless of the type of applied loads (Needleman, 1992). In contrast, potential-based models implement an energy potential function (e.g., polynomial Freed and Banks-Sills, 2008 or exponential Xu and Needleman, 1993) to describe the damage process under displacement jump across the joints, which provides a more realistic methodology for simulating the failure response. A comprehensive review of various cohesive models, together with their applications and limitations is provided in Park and Paulino (2011).

One of the main limitations of phenomenological cohesive laws is the lack of a physics-based description of the damage process, which thus cannot accurately capture the effect of the heterogeneous adhesive microstructure on its failure response. Alternatively, computational cohesive models have recently been implemented to alleviate this limitation by providing a more realistic description of the damage process in different loading conditions and linking the microscopic details of damage to the macroscopic behavior of the structure (Matouš et al., 2008; Kulkarni et al., 2010; Aragón et al., 2013). The derivation of traction-separation laws for multiscale cohesive models relies on computational homogenization techniques (Kanouté et al., 2009). In direct micro-macro homogenization method (Renard and Marmonier, 1987), the constitutive law at each point of the macroscopic model is evaluated by simulating the mechanical behavior of a representative volume element (RVE) of the material assigned to that point (Miehe et al., 1999; 2002; Terada and Kikuchi, 2001; Chen et al., 2014). The so-called FE^2 multiscale method, first introduced by Feyel (1999); Feyel and Chaboche (2000); Feyel (2003), is among the methods adopted for simulating the failure response of adhesive joints (Kulkarni et al., 2010; Hirschberger et al., 2008, 2009). In this method, an RVE is assigned to each quadrature point of finite element mesh discretizing the problem at the macroscopic level and a microscopic simulation is conducted to determine the constitutive behavior of the RVE. Recently, Mosby and Matouš (2014) have developed a hierarchically parallel FE^2 solver for the multiscale cohesive modeling of hyperelastic adhesives using more than one billion elements.

While implementing multiscale methods enables performing high fidelity damage simulations, incorporating the intricate microstructure of the adhesive layer in the computational model remains a challenge. The laborious process of creating realistic geometrical models of the adhesive heterostructure on the one hand and the requirement to generate finite element meshes that match (conform to) materials interfaces on the other hand hinder the straightforward application of the FEM for the treatment of this problem. A similar challenge is observed in simulating the physical behavior of several other materials systems with complex/evolving microstructures, which has led to the development of alternative numerical techniques such as the boundary element method (BEM) (Liu et al., 2011; Wang and Yao, 2013), generalized/extended FEM (GFEM/XFEM) (Oden et al., 1998; Melenk and Babuška, 1996; Duarte et al., 2000; Daux et al., 2000; Sukumar et al., 2000), and interface-enriched generalized FEM (IGFEM) (Soghrati and Geubelle, 2012), Soghrati et al. for the mesh-independent modeling of such problems. The latter two methods rely on enriching the solution field in nonconforming elements cut by the materials interface using the partition of unity (GFEM/XFEM) or generalized interfacial degrees of freedom (IGFEM), which yields a similar performance as the standard FEM but without the need to create conforming FE meshes.

However, even with the aid of methods such as GFEM/XFEM and IGFEM, majority of the former computational studies aimed at quantifying the failure response of adhesives have used simplified microstructural models, often assuming circular/spherical shaped inclusions as embedded particles (Aragón et al., 2013; Mosby and Matouš, 2014). Furthermore, parameters such as pre-existing pores, disbonded regions, and microscopic roughness of adherends surfaces, which can considerably increase the complexity of the computational model, have been overlooked in such studies. Thus, the resulting simulations may not fully capture the impact of the actual complex microstructure of the adhesive layer on the damage process. Note that due to the presence of materials interfaces that are in close proximity or contact in the adhesive microstructure, modeling this problem using GFEM/XFEM or IGFEM can still be challenging. This feature leads to difficulties for evaluating the enrichment functions associated with nonconforming elements cut by multiple materials interfaces, which complicates the implementation of such methods.

Recently, Soghrati (2014) has introduced the hierarchical interface-enriched FEM (HIFEM), which enables the fully mesh-independent modeling and simulation of problems with complex geometries, while yields the same precision and convergence rate as those of the standard FEM. HIFEM implements a straightforward and yet general recursive algorithm for enriching elements cut by an arbitrary number/orientation of materials interfaces, which allows using simple nonconforming structured meshes that are completely independent of the problem morphology for discretizing the domain. This unique advantage considerably automates the modeling process for materials with intricate morphologies, which is an attractive feature for simulating the failure response of heterogeneous adhesives.

The current manuscript aims at quantifying the impact of microstructural features such as the morphology and volume fraction of embedded particles, pores created during the manufacturing process, and adherends surface roughness on the failure response of heterogeneous adhesives. The higher-order HIFEM (Soghrati and Barrera, 2015) is employed to simulate the initiation and progression of damage in the adhesive layer. A new microstructural characterization algorithm is also introduced, which combines the random sequential adsorption (RSA) algorithm (Feder, 1980; Pan et al., 2008; Kari et al., 2007) and the non-uniform rational basis-splines (NURBS) (Piegl and Tiller, 1987; Bhandari et al., 2007) to automatically generate realistic virtual models of the adhesive RVE. We will implement this integrated computational framework to perform a parametric study on the effect of the microstructural features enumerated above on the failure response of an epoxy adhesive with embedded glass particles.

The remainder of this article is structured as follows. Section 2 presents the formulation of the multiscale cohesive model, together with the isotropic damage model used for approximating the failure response of the adhesive. The integrated computational framework developed for the modeling of the adhesive microstructure and the mesh-independent simulation of the damage process is described in Section 3. In Section 4, we study the appropriate size of the RVE for performing damage simulations, followed in Section 5 by investigating the impact of the volume fraction of embedded heterogeneities on the failure response of the adhesive layer. Similar studies on the effects of the voids volume fraction and the adherends surface roughness are presented in Sections 6 and 7, respectively.