



Multiscale simulation of particle-reinforced elastic–plastic adhesives at small strains

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ABSTRACT

Many aerospace, aircraft or automotive mechanical components are joined together by using a structural adhesive. Adherend-to-adherend joint performance is usually carried out by a thin adhesive layer such that loads are transferred through this region, being then a critical point in the design. In order to ensure a proper behaviour of the adhesive under dynamical, mechanical, thermal or rheological loads, they are typically reinforced with a second phase stiffer material in addition to the adhesive matrix. Due to the intrinsic nature of the matrix, it may be approached using an elastic–plastic behaviour. Under these circumstances the adhesive inherently shows a heterogeneous microstructure whereas the loads are applied at the macroscopic adherend scale. In this work, a multiscale formulation is developed to analyze particle-reinforced adhesive joints. The adherend and the adhesive region, which is modelled using cohesive elements, stand macroscopically. On the other hand, the macroscopic adhesive behaviour is obtained by a direct analysis of the two-distinguished phases interaction at the microscopic level, using micromechanics and homogenization. The presented approach provides macroscopic as well as microscopic information about load distribution avoiding phenomenological lab fitting, case to case, of the overall macroscopic behaviour of the adhesive.

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1. Introduction

1.1. Motivation

Since their inception, in the early 1950s, adhesives are widely used in structural applications, most notably in the aerospace, automotive and marine industries replacing traditional mechanical fasteners due to improved load distribution, increased life service, reduced machining cost, and/or reduced complexity [1]. In these applications, an understanding of the material behaviour in the joint is required to optimize design and predict the mechanical performance of the joint in service. Adhesives are physically modified in an attempt to improve their thermal, rheological and mechanical properties. In fact, the use of second phase particles as reinforcement in an otherwise homogeneous adhesive affects the overall material properties such as the elastic modulus, the yield stress and the fracture behaviour. Therefore, many adhesive types are multi-phase segmented polymers that exhibit a two-phase microstructure composed of soft and hard rigid segments [2]. For example, rubber particles [3], natural fibers [4], carbon nanotubes [5,6], glass fibers [7], nanoparticles [2,8,9] and silver flakes [10] have been added to improve the adhesive properties.

Epoxy based adhesives represent the most common type for structural bonding applications. This type of adhesive is also called a toughened epoxy adhesive due to the effect of the second phase added. In fact, when polymerized, epoxy adhesives are amorphous and highly-crosslinked materials and this structure results in many useful properties, such as good thermal stability and creep resistance. However, this also makes the composite brittle and with a poor resistance to fracture and delamination. Thus, a second micro-phase of a dispersed rubbery [11–13] or a thermoplastic polymer [14–16] is incorporated into the epoxy to increase their toughness, without significantly impairing the other desirable engineering properties. To increase further the mechanical performance of these adhesives, small rigid particles [17,18] are also added resulting in hybrid toughened epoxy polymers [19].

There are several factors that could contribute to the failure of two adhered surfaces. The most common types are the cohesive failure, in which failure takes place in the adhesive, and the adhesive failure in which failure between the adhesive and the adherend or substrate occurs. In general, cohesive failure is more common than the adhesive failure. However, these are two of the seven classes of failure modes in adhesive joints, according to the ASTM standard D5573-99, namely, adhesive failure, cohesive failure, thin layer cohesive failure, fibre tear failure, light fibre tear failure, stock break failure and mixed failure. In the cohesive failure, and considering multiphase adhesives, in a first step damage

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starts at the micromechanical level by crack propagation in the matrix phase. After these cracks have grown to a certain length, they interact with each other in a second step, giving rise to a macro-failure of the composite [20]. At the micro level, the strength of the interface inclusion-matrix has a profound effect on the path of the crack around the inclusion [21]. In the case of debonded or poorly-bonded particles, which is similar to that of spherical holes, the maximum tensile stress is at the equators of the particles and holes and the cracks are attracted to the equator of the inclusions. However, if there is a good bonding, the situation is more complex and the maximum stress position is strongly dependent upon the elastic constants of the particles and the matrix [21]. In general, the maximum stresses are in the matrix above and below the poles of the particles and thus the crack runs circumferentially between the inclusions and the matrix. Therefore, to be able to compute the stresses in the matrix and inclusions, which are involved in the mechanism of failure, the model to be developed needs to consider a microscopic formulation.

1.2. Cohesive zone modelling

Several authors have simulated the adhesive interface within the fracture mechanics framework [22–24]. For instance, Andruet et al. [23,24] modelled the adherends with shell elements and the adhesive layer with 3-D solid elements. The modelling was later refined by considering the adhesive layer with shear springs [25–28]. These studies were focused mainly on the macroscopic response of the interface at different loading configurations. However, it is well known that the stress states in the adhesive are definitely more complex and multiaxial in nature.

The fracture process zone can be modelled by non-linear fracture mechanics, e.g. by a cohesive finite element (CFE). This approach, pioneered by Dugdale [29] and Barenblatt [30], has been deeply used during the last two decades (see de Borst et al. [31] for a review) and seems to be well suited to analyze decohesion in composite structures. These models fully represent the mechanical response of the cohesive zone by an appropriate traction–separation relation which provides a phenomenological description for the complex microscopic processes [32–34]. This modelling approach is very attractive since it involves a limited number of parameters, it can easily incorporate mixed mode loading [35–37] and it can consider rate dependent effects [38]. A lot of work has been done for identifying the shape for these traction–separation laws [35,37,39–43]. However, in most cases, the traction–separation relation describing the failure of the adhesive layer is purely phenomenological [44–46]. In addition, the use of a single cohesive zone to describe the entire response of such heterogeneous adhesives remains a strong simplification. Indeed, the mechanisms of cracking of an adhesive layer are very complex, involving multi-axial plastic deformation and various types of damage phenomena developed at different scales. A more versatile model is thus necessary in order to account for at least some of these mechanisms.

1.3. Multiscale approach

Multiscale techniques imply working at two different levels going down and up through the two associated mathematical problems, i.e., *localization* and *homogenization*, respectively. Homogenization strategies are powerful tools to simulate the effective properties of heterogeneous materials (constitutive law) at a very reasonable computational cost. In the framework of linear elasticity, since the pioneering work of Eshelby [47], numerous homogenization schemes have been developed [48–52]. Extensions to non linear materials have been performed by many authors, accounting for thermoelasticity (e.g., [53–55]), plasticity

[56–60], viscoplasticity [61] and damage or porous plasticity [62] amongst others. The accuracy of homogenization models is generally checked through micromechanical modelling approaches which are based on a representative volume element (RVE). RVEs contain enough statistical information about the inhomogeneous medium in order to be representative of the material, allowing modelling complex microstructural geometries and predicting overall composite responses with different geometrical features [63]. Various studies have tried to obtain the effective properties of particle reinforced composites with great accuracy based on finite element simulations of an RVE in the elastic regime [64–66], elastoplastic [67–69], viscoplastic [70] or including the effect of damage by matrix void growth [71,72] and particle fracture [73]. The availability of RVE-based homogenization approaches ultimately depend on RVE size independence, being then necessary the definition of a microscopic characteristic length of the specimen.

A multiscale model able to translate the complex behaviour at the micro level to the macroscopic scale may offer a much realistic approach to define the mechanical performance of the whole composite. To date, limited multiscale modelling frameworks have been developed [74–77]. In the framework of the adhesives, Matous et al. [78] developed a multiscale cohesive model by performing detailed finite element (FE) calculations on the RVE. The main objective of this model was to capture the damage failure on the effective properties. However, this model is of the non-linear elastic type with traction displacement relations which are fully reversible. This leads to inaccurate predictions when plastic deformation occurs, typical for epoxy adhesives. In fact, due to the stress concentrations associated with the small particles, extensive, but localized shear yielding takes place in the matrix. As far as the authors know, no model has yet proposed a micro–macro approach that takes into account plastic deformations in a cohesive model, which has been demonstrated to play an important role in the process of failure of the adhesives.

1.4. Aims and organization of the paper

The aim of this work is to develop a consistent numerical framework for cohesive elements in a multiscale fashion, accounting for plastic strains arising from the adhesive matrix (microstructure). The simulations were carried out within the framework of the finite element method. The results of these novel simulations showed the effect of the dominant deformation and plasticity processes of the adhesive microstructure during loading tests of the composites.

The paper is organized as follows: Section 2 shows the general mathematical modelling at the micro and macro scales. On the other hand, Section 3 provides a comprehensive implementation of the equations introduced in Section 2. Two case problems are highlighted in Section 4 by means of the previously introduced multiscale approach. Finally, the work summary and conclusions are presented in Section 5.

2. General mathematical model

The model consists of two adherends (domain Ω^0) joined by a thin adhesive layer (domain Ω_s^0). The strategy for predicting the behaviour of adhesives used in this work is computational micromechanics, in which the effective properties are obtained from numerical analysis of the mechanical response of an RVE of the microstructure, which explicitly takes into account the spatial distribution of matrix and inclusions. Hereafter we use the superscripts “0” and “1” to represent the macro and micro scales, respectively.

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