International Journal of Solids and Structures 69–70 (2015) 106–120

Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

An anisotropic large displacement cohesive zone model for fibrillar and crazing interfaces

M. Paggi [a,*], J. Reinoso [a,b]

[a] *IMT Institute for Advanced Studies Lucca, Piazza San Francesco 19, 55100 Lucca, Italy*
[b] *Group of Elasticity and Strength of Materials, School of Engineering, University of Seville, Camino de los Descubrimientos s/n, 41092 Seville, Spain*

ARTICLE INFO

Article history:
Received 8 October 2014
Received in revised form 24 January 2015
Available online 10 June 2015

Keywords:
Anisotropic cohesive zone model
Fibrillar interfaces
Large displacements
Photovoltaics
Bonding of paper tissue
Crazing of polymers

ABSTRACT

A new cohesive zone model to describe fracture of interfaces with a microstructurs made of fibrils with statistically distributed in-plane and out-of-plane orientations is proposed. The elementary force–displacement relation of each fibril is considered to obey the peeling theory of a tape, although other refined constitutive relations could be invoked for the adhesive constitutive response without any lack of generality. The proposed consistent 2D and 3D interface finite element formulations for large displacements account for both the mechanical and the geometrical tangent stiffness matrices, required for implicit solution schemes. After a preliminary discussion on model parameters identification, it is shown that by tailoring the spatial density of fibrils at different orientations can be a way to realize innovative interfaces enhancing adhesion or decohesion, depending on the need. For instance, it can be possible to realize microstructured adhesives to facilitate debonding of the glass cover in photovoltaic modules to simplify recycling purposes. Moreover, the use of probability distribution functions describing the density of fibrils at different orientations is a very effective approach for modeling the anisotropy in the mechanical bonding between paper tissues and for simulating the complex process of crazing in amorphous polymers.

1. Introduction

Interfaces with microstructures have been observed in the transition zones between several natural and artificial systems and have been subject of intense research. A pioneering theory of structured interfaces reinforced by fibers modeled as linear elastic bars has been proposed in Bigoni and Movchan (2002) and Bertoldi et al. (2007a,b,c) to deal with interfaces with microstructures like those of the metacarpal bone of a vulture-wing, the pinctada nacre, the short glass–fiber-reinforced polypropylene, the crack tip in polystyrene, the meninges surrounding the human brain, the cross-section of a palm petiole, and the pyrolyzed wood infiltrated with Silicon. The derived results have emphasized the role of the interface microstructure on the properties of a linear elastic system, both in statics and in dynamics.

Along this line of research, attempts to describe the nonlinear behavior of finite thickness interfaces by developing synthetic traction-inelastic separation relations, or cohesive zone models, have been proposed in Paggi and Wriggers, 2011a,b, 2012 for polycrystalline materials, explicitly considering the evolution of damage in these finite thickness regions. A different set of computational approaches, that aim at providing a further insight into the fibrillation using micromechanics-based models and including viscoelastic effects, has been developed in Allen and Searcy (2001) and Estevez et al. (2000), among others. As an alternative route, multi-scale computational methods have been proposed in Matous et al. (2008) to derive the cohesive zone model response of particle reinforced adhesives by a multi-scale analysis explicitly taking into account the finite element representation of the interface microstructure. Geers and coworkers (van den Bosch et al., 2008b; Vossen et al., 2014) have also recently developed a multi-scale strategy to simulate the mechanism of fibrilation in the delamination of polymer-coated metal sheets. These investigations are based on a series of experimental works devoted to the understanding of the fibrillation processes in polymers (see Kramer and Berger (1990), Creton and Lakrout (2000), Hoefnagels et al. (2010), Desai et al. (2011) and the references therein given) which basically regard: (1) the voids formation along the interface, (2) the generation of load bearing crazes (fibrils), and (3) the final failure of such fibrils, leading to interface crack propagation.

In parallel with these studies, mostly dealing with fracture of imperfect finite thickness interfaces joining dissimilar materials,

---

* Corresponding author. Tel.: +39 0583 4326 604; fax: +39 0583 4326 565.
E-mail addresses: marco.paggi@imtlucca.it (M. Paggi), jreinoso@us.es (J. Reinoso).

http://dx.doi.org/10.1016/j.ijsolstr.2015.04.042
0020-7683/© 2015 Elsevier Ltd. All rights reserved.

another impressive line of research has focused during the last decade on the morphology of surfaces of living systems and its connection with their adhesion capabilities. The analysis of pads and surfaces of insects, spiders and lizards have revealed the presence of a complex texturing able to maximize adhesion and tolerate interfacial crack-like flaws caused by surface roughness (Gao et al., 2004; Yao and Gao, 2008). A notable example are the pads of Tokay gecko, showing a hierarchical assembly of microscale hairs, called *setae*, branching off into nanoscale *spatulae* (Huber et al., 2005; Scherge and Gorb, 2001; Pugno and Lepore, 2008; Pugno et al., 2011; Lepore et al., 2012). Extensive modeling of the gecko attachment/detachment system has provided a valuable insight into the mechanisms promoting the adhesion of natural and bio-inspired interfaces (Gao et al., 2005; Yao and Gao, 2007; Yao et al., 2008). At the microscale, the adhesive behavior of spatulae has been successfully modeled as an elastic tape (Gao et al., 2005), conforming with the semi-analytical adhesion theory by Kendall (1975). The ability to tolerate roughness was finally explained by a hierarchical assembly of fractal type of spatulae and hairs (Yao and Gao, 2006, 2008). Moreover, for releasable adhesion, the macroscopic elastic anisotropy was found to vary the adhesion strength significantly with the direction of pulling, leading to an orientation-controlled switch between attachment and detachment scenarios (Yao and Gao, 2006; Chen and Gao, 2007; Chen et al., 2008).

The bottom-up design principles of structured interfaces and surfaces emerging from the aforementioned state-of-the-art on the subject open a frontier of research in the design of novel adhesives for a wide range of engineering applications. In the present work, an anisotropic interface constitutive law based on the adhesion mechanisms of fibrils at the microscale is proposed. The key idea is to derive a traction-separation law or cohesive zone model (CZM) based on bottom-up considerations. The interface region is modeled at the micro-scale as a surface covered by fibrils adhering to a substrate with certain in-plane and out-of-plane orientations. The force–elongation relation of each fibril will provide an elementary contribution to the overall cohesive traction-separation relation of the interface resulting from their spatial integration. As a result of the orientation-dependent tractions stemming from the classical equations of the peeling theory proposed by Kendall (1975), this basic model will provide an adhesion force dependent on the mode of deformation experienced by the interface. This formulation is further enhanced by showing that a possible way to maximize or minimize adhesion along specific directions can be achieved by introducing a probability distribution function to describe the density of fibrils with a given inclination, instead of assuming a uniform distribution. From the numerical standpoint, within the context of nonlinear FEM, the 2D and 3D versions of the adhesion/decohesion model herein proposed is incorporated into the large deformation interface element recently developed in Reinoso and Paggi (2014), providing a robust and versatile computational framework for engineering simulations.

The paper is organized as follows. Section 2 is concerned with the formulation of an anisotropic cohesive zone model that accounts for interfaces with a microstructural arrangement based on fibril distributions for 2D and 3D applications. Since the developed model is expected to have a special impact on maximizing adhesion or detachment of thin-walled structures undergoing large-displacements, details concerning the 3D generalization of the novel interface element formulation proposed in Reinoso and Paggi (2014) are given in Section 3. This interface element provides a consistent derivation to deal simultaneously with material and geometrical nonlinearities in those detachment applications where both nonlinearities have a relevant role. Using this computational method, applications related to the understanding of the behavior of cellulose fibrils in paper tissue bonding, and a new possibility to facilitate disassembling operations in photovoltaic modules for recycling purposes are investigated in Section 4. Finally, the main conclusions of the present contribution along with its further potential capabilities are addressed in Section 5.

2. Derivation of the anisotropic cohesive zone model: adhesion control based on the peeling theory

In this section the anisotropic interface constitutive relation based on the peeling theory for controlling the adhesion of interfaces with a fibrillar microstructure is derived. After introducing a two-dimensional formulation, its generalization to three-dimensional problems is presented. The corresponding mathematical treatments are kept separate in this section since they have different degrees of complexity as far as the finite element implementation detailed in Section 3 and in Appendix is concerned.

2.1. Two-dimensional constitutive model

Let assume the microstructural arrangement of the interface be covered by a collection of elastic fibrils or spatulae perfectly joined to the body sharing the upper side of the interface and bonded to the opposite side as an adhesive tape, see Fig. 1. Introducing as customary a local reference system defined by the tangent and normal vectors to the middle-line of the interface, which is updated during the deformation process, these fibrils may have different instant inclination angles β, possibly covering all the values ranging from zero to π.

Regarding the initial value of the angle β, different options may be considered. When a surface is adhering on a substrate by the action of fibrils, as in Fig. 1, their inclination angle can obey a statistical distribution. For instance, groups of polymer chains bridging a crazing crack may have a uniform distribution of orientations, see e.g. Fig. 2.

In case of hairy pads of living insects or Gecko's spatulae, the angle β is in general different from zero and it is influenced by the statistics of surface texturing and roughness which govern the contact angles with the spatulae. As recently investigated in Zhou et al. (2014), the angle β can have a deterministic value only if the texturing is regular as in the form of cylinders, see Fig. 3(a), or in case of sinusoidal waviness as considered in Gillies and Fearing (2014). In the more general case of random roughness, a statistical distribution of angles β is expected to arise from the actual distribution of the local slopes of the profile height field. As an example, the probability distribution density function of angles β computed from the statistical analysis of the profiles of a fractal surface with $D = 2.3$ and generated with the random midpoint displacement algorithm is shown in Fig. 3(a), and it resembles a Gaussian distribution.

We also admit the possibility to have a nonuniform distribution obtained from the subtraction of a Gaussian distribution from a uniform distribution. This can be used to model an interface with a reduced density of fibrils centered around a given orientation. The resulting probability distribution function will present a reduced frequency of fibrils along the pre-selected orientation, thus weakening adhesion along that specific direction. This configuration will be referred to as *nonuniform distribution for detachment* in the sequel.

In summary, with the aim of accounting for the initial microstructural arrangement of interfaces based on fibril distributions, we propose the introduction of a factor $a_f(\beta)$ that will provide the frequency of fibrils with an initial out-of-plane inclination β: