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Multiscale analysis of mixed-mode fracture and effective traction-separation relations for composite materials

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ABSTRACT

A multiscale framework for the analysis of fracture is developed in order to determine the effective (homogenized) strength and fracture energy of a composite material based on the constituent's material properties and microstructural arrangement. The method is able to deal with general (mixed-mode) applied strains without a priori knowledge of the orientation of the cracks. Cracks occurring in a microscopic volume element are modeled as sharp interfaces governed by microscale traction-separation relations, including interfaces between material phases to account for possible microscale debonding. Periodic boundary conditions are used in the microscopic volume element, including periodicity that allows cracks to transverse the boundaries of the volume element at arbitrary orientations. A kinematical analysis is presented for the proper interpretation of a periodic microscopic crack as an equivalent macroscopic periodic crack in a single effective orientation. It is shown that the equivalent crack is unaffected by the presence of parallel periodic replicas, hence providing the required information of a single localized macroscopic crack. A strain decomposition in the microscopic volume element is used to separate the contributions from the crack and the surrounding bulk material. Similarly, the (global) Hill–Mandel condition for the volume element is separated into a bulk-averaged condition and a crack-averaged condition. Further, it is shown that, though the global Hill–Mandel condition can be satisfied a priori using periodic boundary conditions, the crack-based condition can be used to actually determine the effective traction of an equivalent macroscopic crack.

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1. Introduction

Prediction of the onset and evolution of failure in composite materials such as fiber-reinforced composites is an essential factor in the design and development of load-bearing components used in lightweight structures. While significant progress has been achieved in this area since the transportation industry embraced the use of composites, there is a need to further refine the predictability and robustness of models used to analyze failure. Current safety factors used in design of structures made of composite materials significantly limit their efficiency due to large uncertainties. Multiscale methods offer the possibility of incorporating detailed information of a composite, which should lead to an improvement in accuracy of failure models. Equally important is the need to develop models that predict the evolution of failure in composites, which

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is relevant in order to determine the residual structural strength after (partial) failure or to design a structure against a catastrophic event (e.g., impact).

In recent years, the use of cohesive laws, in conjunction with either cohesive elements or with the extended finite element method (XFEM) has gained popularity as a tool to simulate the onset and propagation of cracks in composite materials. Nevertheless, establishing reliable cohesive laws for composite materials remains challenging, particularly regarding the incorporation of lower length scale information at a higher length scale. The determination of a macroscopic cohesive relation, which accounts for microscale features and fracture mechanisms, relies on a homogenization approach that translates the detailed behavior in a microstructural volume element into an effective (macroscale) response. For multiscale formulations involving fracture, the classical notion of a representative volume element (RVE) that is based on a continuous displacement requires a modification (see, e.g., Gitman et al., 2007). An alternative averaging formulation based on a damaged zone within the volume element was proposed by Nguyen et al. (2010) where it was concluded that with a proper identification an RVE can be established.

Multiscale formulations have been applied to the so-called adhesive cracks, in which it is a priori known in what region and, more importantly, in what orientation a macroscopic crack is expected to nucleate and grow (Kulkarni et al., 2010; Matous et al., 2008; Verhoosel et al., 2010). Micromechanical formulations have been used to study failure in polymer composites using periodic boundary conditions in Melro et al. (2013) where the influence of the distinct material and interface properties were analyzed. Similarly, the influence of defects on the strength and fracture energy of a fiber-reinforced unidirectional composite under extension was analyzed in Alfaro et al. (2010b) where it was observed that imperfections may increase the effective crack length compared to the crack length in a sample without imperfections, thus actually increasing the macroscopic fracture energy. In-plane periodic conditions were used to analyze the response of one ply in Arteiro et al. (2014), with elastic adjacent plies preventing out-of-plane crack propagation beyond the ply analyzed (i.e., a so-called “wall effect” as described in Gitman et al., 2007). Their simulations provide insight on the interplay between ply geometry and properties, constraining effects of adjacent plies and the resulting crack patterns.

One issue that has been identified as a potential problem is related to the strong (i.e., pointwise) periodic boundary conditions and its effect on the results. To overcome the limitation of having to prescribe a priori the orientation of a crack (i.e., analysis limited to adhesive cracks) and simultaneously to address some doubts that have been raised about the suitability of strong periodic boundary conditions to analyze fracture, a multiscale transition scheme was proposed in which the representative volume element is, upon the onset of cracking (localization of damage), replaced by a microstructural volume element (MVE) (Bosco et al., 2015; Coenen et al., 2012a; 2012b). Through a continuous adaptation of the loading at the microscale level, using the so-called percolation-path-aligned boundary conditions, the MVE provides a macroscopic response aligned with the average orientation of the crack as it develops throughout the loading process. Their scheme was implemented in a so-called FE^2 framework, where numerical simulations are simultaneously conducted at the micro and macroscales. Also addressing the issue of strong periodic boundary conditions, an alternative approach pertaining to weakly periodic boundary conditions has been recently developed (Svenning et al., 2016a; 2016b). These conditions lead to a mixed traction-displacement formulation as unknowns in the boundary.

The FE^2 approach requires continuous bi-directional exchange of information between the macroscale and the microscale domains throughout a simulation (Mosby and Matous, 2016). In a displacement-driven multiscale formulation, a macroscale strain increment is given as input to an RVE (in undamaged zones) or to an MVE (in damaged areas) and the corresponding microscale boundary value problem is solved, which explicitly accounts for microstructural phenomena. Subsequently, the averaged microscale response is provided as input to the macroscale boundary value problem, typically in the form of an average (macroscopic) stress increment, a tangent (value of derivative of stress with respect to a strain measure) and possibly some variables that are treated as internal parameters at the macroscale. In this approach, the constitutive information at the macroscale is not specified in closed-form (or with a system of equations) but rather in implicit form through the (incremental) solution of microscale boundary value problems, one for each macroscale integration point in a finite element formulation.

An alternative approach, which is attractive from the point of view of computational efficiency, is to propose a macroscopic model in closed-form and use MVEs to essentially calibrate the constitutive information a priori (i.e., the parameters in the macroscopic model are chosen to approximate the explicit MVE results). The clear advantage is that it is possible to carry out a single-scale computation while retaining relevant information about the microscale phenomena. One limitation of this approach is that the macroscopic model may not be able to reproduce all possible responses from the MVE calculation, particularly for complex loading histories. Nonetheless, accurate results may be expected for simpler loading cases (e.g., locally proportional loading), which can still reproduce a relatively complex macroscopic loading case.

Within the context of computational efficiency, the present work addresses two issues in a hierarchical multiscale framework for fracture: (i) the suitability of strong periodic boundary conditions under relatively general loading conditions and (ii) a methodology to establish a macroscopic cohesive law that implicitly incorporates microscopic information. For the first issue, an analysis is carried out to introduce the notion of an “equivalent crack domain”, where it is shown that the response after localization due to fracture under strong periodic boundary conditions can be described by a single equivalent crack and is independent of parallel crack replicas. The method relies on a description of fracture at the microscale level based on crack surfaces (as opposed to distributed damage theories that simulate cracking in a region). In practice this simplifies the numerical implementation since only one type of fracture model is required. Furthermore, the crack surface approach can still be used in conjunction with a distributed model for, e.g., plasticity. Through representative simulations it

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