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ScienceDirect
Comput. Methods Appl. Mech. Engrg. 196 (2006) 620–633
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Finite element formulation for modeling particle debonding in reinforced elastomers subjected to finite deformations ☆

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Received 20 July 2005; accepted 9 June 2006

Abstract

Interfacial damage nucleation and evolution in reinforced elastomers is modeled using a three-dimensional updated Lagrangian finite element formulation based on the perturbed Petrov–Galerkin method for the treatment of nearly incompressible behavior. The progressive failure of the particle–matrix interface is modeled by a cohesive law accounting for mode mixity. The meso-scale is characterized by a unit cell, which contains particles dispersed in a homogenized blend. A new, fully implicit and efficient finite element formulation, including consistent linearization, is presented. The proposed finite element model is capable of predicting the non-homogeneous meso-fields and damage nucleation and propagation along the particle–matrix interface. Simple deformations involving an idealized solid rocket propellant are considered to demonstrate the algorithm.

Keywords: Decohesion; Cohesive and volumetric elements; Stabilized method; Finite deformations; Particulate composites

1. Introduction

With examples ranging from automobile tires to solid propellants, particle-reinforced elastomers play an important role in a wide variety of engineering applications and the modeling of their constitutive response continues to be a long-standing research topic. The complexity of the modeling is associated with the combination of a large set of sometimes competing physical processes taking place at various length scales: large deformations of the quasi-incompressible elastomeric matrix, large stiffness mismatch between the matrix and the reinforcing particles, non-linear viscoelastic response of the elastomer, Mullins hysteretic effect under cyclic loading, particle debonding, void growth, matrix tearing, inter-particle interaction, etc.

The number and complexity of these phenomena have led most of the modeling efforts reported in the literature to rely on homogenized continuum models to capture some of these key features of the mechanical response. For example, Bergstrom and Boyce [2] have proposed a dual-network model to predict the non-linear viscoelastic response of carbon-black reinforced rubbers, with emphasis on capturing the large deformation and Mullins effects. Drozdov and Dorfmann [8] also used the network theory of rubber elasticity to capture the non-linear equilibrium response of filled and unfilled elastomers. Most theories, however, are based on phenomenological continuum models of various features of the constitutive response of filled elastomers. Examples include Dorfmann and Ogden's analysis of the Mullins effect [7], Kaliske and Rothert's work on the internal friction [13] and Miehe and Keck's stress decomposition model of damage evolution [25].

Another complexity is associated with the numerical treatment of these materials. As mentioned earlier, the matrix material is nearly incompressible and a special numerical formulation has to be employed. A mixed finite element method that interpolates the pressure and displace-

☆ US Department of Energy, B341494.
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doi:10.1016/j.cma.2006.06.008

ment fields separately is required. For Galerkin methods, the choice of interpolation functions must satisfy the Babuška–Brezzi condition (see, e.g., [4]) in order to achieve uniqueness, convergence and robustness. Without balancing the interpolations properly, significant oscillations in the solution typically result. Considerable effort has been devoted in recent years to develop novel numerical techniques that give stable solution [23,37,5]. Especially, stabilized theories, where Babuška–Brezzi stability condition is circumvented, have been recently explored [16,17,27].

The primary focus of this research is to develop a computational model of damage evolution under high strain levels in highly filled elastomers such as solid propellants and other energetic materials, which are composed of particles of varying sizes (typically a bimodal distribution) needed to achieve a high energetic content. Various "homogenized" models have been proposed to simulate the damage evolution: see, for example, the analysis presented by Farris [11], Schapery [33], Ha and Schapery [14], Simo [36], Ravichandran and Liu [30]. Other approaches rely on micromechanics [22,18,38].

In these highly filled elastomers, experimental observations have shown that the failure process is primarily driven by the debonding of the larger particles, with the smaller particles playing the role of stiffener for the matrix [1,29]. Based on these observations, Zhong and Knauss [44,45] have used a cohesive finite element approach to simulate the progressive particle debonding process in simple 2D representative volume elements (RVE) composed of a few large rigid particles embedded in a non-linear elastic matrix. The emphasis of their work was to capture the effect of the inter-particle interaction and the influence of the interface cohesive properties on the evolution and stability of the dewetting process.

Building on Zhong and Knauss' work, we present a numerical study where the key emphases are: (1) the development and implementation of a 3D model under large deformations; (2) the accurate and efficient treatment of the near-incompressibility of the matrix through a stabilized finite element formulation; (3) the consistent linearization of the set of non-linear equilibrium equations leading to a very efficient algorithm.

In this paper, the interfacial damage is modeled by cohesive elements [28,31,12,43] and the stabilized Petrov–Galerkin formulation is used to describe the large incompressible deformations of a matrix [16,17]. The formulation and implementation of the mathematical theory of homogenization in finite strains is presented in paper by Matouš and Guebelle [24]. The presented work can also serve as a computational component in the embedded multiscale scheme proposed by Oden [26] for example.

The paper is organized as follows: In Section 2, we summarize the basic kinematic, equilibrium and constitutive relations that describe the problem, including the cohesive model characterized by an exponential traction–separation law that accounts for mode mixity. A stabilized variational framework based on an updated Lagrangian formulation is presented in Section 3, together with the finite element formulation and its consistent linearization. Section 4 describes constitutive laws characterizing the mechanical behavior of individual constituents. A few comments about the non-linear solver and an adaptive time stepping procedure are presented in Section 5, together with a few illustrative example involving the uniaxial loading of simple unit cells composed of one and four reinforcing particles.

The symbolic notation adopted herein uses upper case boldface italic and lower case boldface Greek letters, e.g., $\boldsymbol{P}$ and $\boldsymbol{\sigma}$ for second-order tensors. The trace of the second-order tensor is denoted as $\mathrm{tr}(\boldsymbol{A})$, and the tensor operations between two second-order tensors $\boldsymbol{S}$ and $\boldsymbol{E}$ are indicated as $\boldsymbol{SE}$ for a tensor contraction (a second-order tensor) or $\boldsymbol{S}:\boldsymbol{E}$ for the scalar product (a double contraction).

2. Finite strain irreversible cohesive law

Consider a hyperelastic body in an initial configuration $B_0 \subset \mathbb{R}^3$, which undergoes the motion $\boldsymbol{\phi}(\boldsymbol{X}, t)$ and let $\boldsymbol{F}(\boldsymbol{X},t) = \nabla\boldsymbol{\phi}(\boldsymbol{X},t)$ be the deformation gradient at the current time $t \in \mathbb{R}^+$ with the Jacobian given by $J = \det(\boldsymbol{F})$. Here $\boldsymbol{X} \in \mathbb{R}^3$ designates the position of a particle in the reference configuration $B_0 \subset \mathbb{R}^3$ in the Cartesian coordinate system. Suppose now that the body is divided by a cohesive surface S_0 with a unit normal $\boldsymbol{N}_0$ (Fig. 1). For the sake of simplicity, we assume that the cohesive surface partitions the body into two subbodies $B_0^{\pm}$, occupying the plus and minus sides of the cohesive surface, $S_0^{\pm}$, respectively.

Next, let $\boldsymbol{x} = \boldsymbol{\phi}(\boldsymbol{X},t)$ be the spatial coordinates of a particle and $\boldsymbol{x}_{n+1} = \boldsymbol{X} + \boldsymbol{u}_{n+1}$, where $\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \boldsymbol{u}$ denotes the incremental displacement field. Here and henceforth, right subscripts n and $n+1$ indicate times t_n and t_{n+1}, respectively. Using an *updated Lagrangian* formulation and adopting the multiplicative decomposition of the deformation gradient, we arrive at

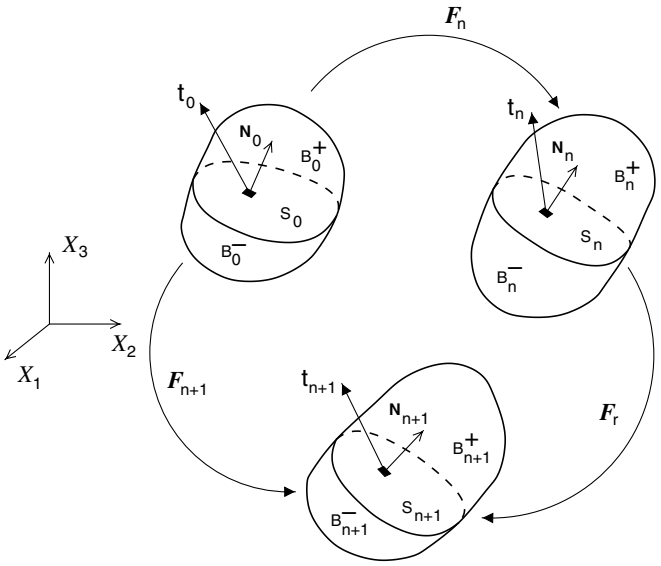

Fig. 1. Kinematic decomposition of deformation gradients.