Journal of the Mechanics and Physics of Solids 65 (2014) 93–113

Contents lists available at ScienceDirect

Journal of the Mechanics and Physics of Solids

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

Phase field modeling of fracture in rubbery polymers. Part I: Finite elasticity coupled with brittle failure

Christian Miehe [*], Lisa-Marie Schänzel

Institute of Applied Mechanics (CE), Chair I, University of Stuttgart, Pfaffenwaldring 7, 70550 Stuttgart, Germany

ARTICLE INFO

Article history:
Received 23 November 2012
Received in revised form
6 May 2013
Accepted 20 June 2013
Available online 31 July 2013

Keywords:
Rubbery polymers
Fracture
Phase field modeling
Finite strain
Coupled multi-field problem

ABSTRACT

This work presents a new phase field model for rate-independent crack propagation in rubbery polymers at large strains and considers details of its numerical implementation. The approach accounts for micro-mechanically based features of both the elastic bulk response as well as the crack toughness of idealized polymer networks. The proposed *diffusive* crack modeling based on the introduction of a crack phase field overcomes difficulties associated with the computational realization of *sharp* crack discontinuities, in particular when it comes to complex crack topologies. The crack phase field governs a crack density function, which describes the macroscopic crack surface in the polymer per unit of the reference volume. It provides the basis for the constitutive modeling of a degrading free energy storage and a crack threshold function with a Griffith-type critical energy release rate, that governs the crack propagation in the polymer. Both the energy storage as well as the critical energy release due to fracture can be related to classical statistical network theories of polymers. The proposed framework of diffusive fracture in polymers is formulated in terms of a rate-type variational principle that determines the evolution of the coupled primary variable fields, i.e. the deformation field and the crack phase field. On the computational side, we outline a staggered solution procedure based on a one-pass operator split of the coupled equations, that successively updates in a typical time step the crack phase field and the displacement field. Such a solution algorithm is extremely robust, easy to implement and ideally suited for engineering problems. We finally demonstrate the performance of the phase field formulation of fracture at large strains by means of representative numerical examples.

1. Introduction

The prediction of failure mechanisms due to crack initiation and propagation in rubber-like materials is of great importance for engineering applications. Practical applications are the modeling of fracture phenomena in tires, seals, medical devices, conveyor belts and base isolations of buildings. A rubbery polymer may exhibit a very complicated inelastic behavior at finite strains. Besides its complex highly non-linear elasticity, complicated inelastic features such as visco-elastic-plastic phenomena and the so-called Mullins' effect of strain-softening occur, see for example Miehe and Keck (2000) and references cited therein for a purely macroscopic account. In this first part of our work on fracture in rubbery polymers, we focus on crack propagation in rubbers with an *idealized purely elastic response*. This is typically achieved for very *slow deformation processes*, where viscous effects can be neglected. For this scenario, we outline a new phase field approach to crack propagation, which embeds micro-mechanically based network theories of both the elastic bulk response as well as the crack toughness.

---

[*] Corresponding author. Tel.: +49 711 685 66379; fax: +49 711 685 66347.
E-mail addresses: christian.miehe@mechbau.uni-stuttgart.de, cm@mechbau.uni-stuttgart.de (C. Miehe).
URL: http://www.mechbau.uni-stuttgart.de/ (C. Miehe).

0022-5096/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jmps.2013.06.007

1.1. *Elastic bulk response of rubbery polymers at finite strains*

The *elastic bulk response* of rubbery polymers is dominated by an extreme reformability and can be well explained by statistical micro-mechanics, see for example Treloar (1975) for an introduction. Rubber elasticity is achieved by a molecular micro-structure consisting of very flexible and mobile long chain molecules and a three-dimensional network that is formed by occasional cross-links between molecules. The dominant contribution to the elastic response of rubber-like materials is due to changes in conformations of network constituents, yielding the so-called entropy elasticity theory. Entropic elasticity of chain molecules is well established in the context of statistical mechanics, see Kuhn (1934, 1936), Kuhn and Grün (1942), Treloar (1975), Flory (1989) and references cited therein. In the literature, many constitutive models for the macroscopic elastic response of rubbery polymers have been developed, see Boyce and Arruda (2000) and Miehe et al. (2004) for an overview. *Purely phenomenological macro-models* involve invariant or principal stretch based isotropic free energy functions, often having polynomial structures. The most advanced formulations are those of Ogden (1972, 1984). However, these approaches lack relations to the molecular structure of the material. This is achieved by *micro-mechanically based network models*, such as the three chain model proposed by James and Guth (1943), the eight chain model suggested by Arruda and Boyce (1993) and the affine full network models considered in Treloar (1946), Treloar and Riding (1979) and Wu and van der Giessen (1993). It is well-known that the affinity assumption between microscopic and macroscopic deformation is not in agreement with experimental observations, in particular in the range of large deformations. Consequently, Boyce and Arruda (2000) argued that the eight chain model yields more realistic results than the seemingly more precise affine full network models. A further improvement provides the non-affine micro-sphere model proposed in Miehe et al. (2004), which allow a flexible modeling of the locking stretches in multi-dimensional deformations. The above mentioned micro-mechanically based models consider idealized polymer networks with free motions of its single chains. However, in real networks topological constraint effects arise due to entanglement-like formations. Molecular-based statistical approaches that incorporate these effects are *constrained junction theories* which formulate the topological constraints around the junctions and the *constrained segment theories*. The constraint junction part of the model proposed by Flory and Erman (1982) was used by Boyce and Arruda (2000) to improve the performance of the eight chain model. The constraint segment approach is consistent with the so-called tube models of rubber elasticity, see for example Deam and Edwards (1976), Edwards and Vilgis (1988), Heinrich and Straube (1983) and Heinrich and Kaliske (1997). In Miehe et al. (2004), we equipped the micro-sphere model with a characteristic micro-tube deformation that is linked to the macroscopic deformation. This microsphere model with a low number of physically based material parameters shows an excellent fit to experimental results. The phase field model of fracture in polymers developed in this work allows the *incorporation of all the above mentioned models* for the bulk response rubbers.

1.2. *Fracture toughness of rubbery polymers at finite strains*

Similar to the elastic bulk response, the *fracture toughness* of rubbery polymers can be rooted in statistical micro-mechanics. The occurrence of macroscopic fracture of rubbery polymers is a result of the failure of the network at the molecular level. When a rubber-like material is deformed, the network constituents change their conformation and polymer chains align according to the above mentioned bulk models. At a critical load level, rupture of one first molecule occurs, inducing the overload and breakage of neighboring chains. Further loading of the body involves rupture of additional chains and finally a macroscopic crack is generated. Early investigations of failure of rubbers were performed in a sequence of papers by Rivlin and Thomas (1953), Thomas (1955), Greensmith and Thomas (1955) and Greensmith (1956). Here, a *critical macroscopic fracture toughness or tearing energy for rubbers* was defined in the sense of a critical energy release rate in line with the classical approach to fracture by Griffith (1920). In a pioneering work, Lake and Thomas (1967), explained these experimental observations by a simple *molecular-theoretical model*, which determines this critical surface energy in terms of the parameters of the network. It turned out that the energy to create a new crack surface predicted by this micro-mechanical model is much less than the tearing energy measured in the above mentioned works. The difference can be explained by *additional dissipative mechanisms* in the material that surrounds the crack tip, see for example Persson et al. (2005) for a recent review. Energy dissipation at the advancing crack in a viscoelastic solid has two contributions. The first is associated with the *innermost region at the crack tip*, where a new macroscopic crack surface is created by chain pull out and bond breaking. This contribution is related to the basic molecular strength of the material and the theoretical prediction of Lake and Thomas (1967). The second contribution comes from the viscoelastic dissipation in front of the crack tip, see for example Persson and Brener (2005) and Kroon (2011). This implies that the critical tearing energy of rubber depends strongly on both the temperature as well as the crack tip velocity. However, as noted by Ahagon and Gent (1975), a reasonable good agreement with the theoretical results of Lake and Thomas (1967) can be obtained in experimental measurements under near equilibrium conditions, such as reported in Mueller and Knauss (1971). They succeeded in measuring low tearing energies, independent of the rate of crack propagation and temperature, by employing low rates of tear.In this first part of the work, we focus on such a scenario and *neglect viscoelastic effects*.

1.3. *A phase field modeling approach to brittle fracture*

The recent works Miehe et al. (2010a, 2010b) outline a general thermodynamically consistent framework for the *phase field modeling of crack propagation at small-strains*. The formulation is essentially a gradient damage theory, however, with critical ingredients rooted in fracture mechanics. This concerns in particular the introduction of a *crack surface density function* $\gamma_l(d, \nabla d)$,