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A theory for fracture of polymeric gels

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ABSTRACT

A polymeric gel is a cross-linked polymer network swollen with a solvent. If the concentration of the solvent or the deformation is increased to substantial levels, especially in the presence of flaws, then the gel may rupture. Although various theoretical aspects of coupling of fluid permeation with large deformation of polymeric gels are reasonably well-understood and modeled in the literature, the understanding and modeling of the effects of fluid diffusion on the damage and fracture of polymeric gels is still in its infancy. In this paper we formulate a thermodynamically-consistent theory for fracture of polymeric gels – a theory which accounts for the coupled effects of fluid diffusion, large deformations, damage, and also the gradient effects of damage. The particular constitutive equations for fracture of a gel proposed in our paper, contain two essential new ingredients: (i) Our constitutive equation for the change in free energy of a polymer network accounts for not only changes in the entropy, but also changes in the internal energy due to the stretching of the Kuhn segments of the polymer chains in the network. (ii) The damage and failure of the polymer network is taken to occur by chain-scission, a process which is driven by the changes in the internal energy of the stretched polymer chains in the network, and not directly by changes in the configurational entropy of the polymer chains. The theory developed in this paper is numerically implemented in an open-source finite element code MOOSE, by writing our own application. Using this simulation capability we report on our study of the fracture of a polymeric gel, and some interesting phenomena which show the importance of the diffusion of the fluid on fracture response of the gel are highlighted.

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1. Introduction

There are numerous polymeric materials which have a crosslinked network and which can absorb large quantities of suitable fluids without the essential skeletal network structure of the polymer being disrupted by the absorbed fluid. Such a polymeric network, together with the fluid molecules, forms a swollen aggregate called a polymeric gel. When the fluid is water, the gel is known as a hydrogel. Gels may be designed to swell by several hundred percent, and – depending on the precise constitution of a gel – the amount of swelling may be controlled by varying external stimuli. Stimuli-responsive polymeric gels have the ability to swell and deswell in response to changes in the environmental conditions such as mechanical forces, temperature, solvent-type, pH, electric field, and also light. Because of their unique characteristics, polymer gels are found in several diverse applications, such as carriers for drug delivery, scaffolds for tissue engineering, soft actuators, smart optical systems, as well as packers for sealing in oil-wells. Living organisms are largely made of polymer gels;

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this facilitates the transport of ions and molecules within the organism while keeping its solidity (shape). Hydrogels are commonly considered as proxies for soft biological tissues and are thus the subject of intense theoretical and experimental investigations.

There have been several (essentially-similar) recent publications regarding modeling of the coupled diffusion-deformation response of polymeric gels (Chester and Anand, 2010; Doi, 2009; Duda et al., 2010; Hong et al., 2008). Several papers related to the numerical implementation of these theories for solving coupled diffusion-deformation boundary value problems for gels have also been recently published (Broger et al., 2017a; Chester and Anand, 2011; Chester et al., 2015; Lucantonio et al., 2013).

In order to develop a robust simulation capability for the use of polymer gels in applications, one also needs to be able to model the damage and fracture of these materials. A difficulty in modeling the fracture of gels comes from the influence of the amount of fluid on the propensity to fracture of a gel. Generally, an inhomogeneous deformation field induces an inhomogeneous chemical potential field, which leads to an inhomogeneous concentration of the fluid because of diffusion within the body; such an inhomogeneous fluid concentration leads to an inhomogeneous propensity to fracture within the body. According to the classical arguments of Lake and Thomas (1967), regions of higher fluid concentration (and therefore lower polymer volume fraction) have an increased propensity to damage and failure because of the lower number of highly stretched polymer chains. Further, because of the diffusion, the damage process zone in the vicinity of a crack – when compared to the overall geometry of a body – is not always small, and classical notions of “small-scale process zone” often do not hold. The heterogeneous propensity to fracture and large damage process zones makes classical fracture mechanics criteria – like the energy release rate reaching a critical value – inapplicable. Also, since diffusion of the fluid relative to the polymer network is a dissipative process, classical fracture mechanics models which are based entirely on Lake–Thomas-type energetic arguments, and which do not account for the dissipation due to diffusion, will underestimate the fracture resistance of polymeric gels.

Thus a theory and a numerical simulation capability which couples diffusion of the fluid with the large deformation, damage and fracture of polymeric gels is needed. Most of the existing studies on the fracture of gels have limited their attention to conditions under which the characteristic time-scale for deformation is much smaller than the time-scale for diffusion, so that the diffusion of the fluid may be neglected (Brown, 2007; Tanaka, 2007; Zhang et al., 2015). However, there are many important operating conditions under which the fluid diffusion cannot be ignored. One such set of conditions occurs when a notched-specimen is stretched to a sub-critical level and thereafter the stretch is held constant; after a sufficient incubation time damage initiates, accumulates, and eventually fracture occurs – a phenomenon known as “delayed-fracture”; this phenomenon cannot be explained by ignoring the diffusion of the fluid (Bonn et al., 1998; Tang et al., 2017; Wang and Hong, 2012).

There are very few papers in the literature which address the complete coupled diffusion-deformation-fracture problems in gels; the only paper that we are aware of is the very recent paper of Broger et al. (2017b). In their paper these authors propose a diffusion-deformation-fracture theory with a diffuse-crack approximation based on a phase-field/damage variable d .¹ They present a variational framework for their phase-field fracture theory of gels together with a numerical implementation of their variational theory in a finite element program, and show some interesting simulations of crack initiation and propagation during drying of hydrogels. For other previous papers on fracture of polymer gels – papers which are based on generalizations of classical fracture mechanics theories and not on phase-field or gradient-damage theories – see, e.g., Wang and Hong (2012), Hui et al. (2013), Bouklas et al. (2015), and Noselli et al. (2016).

The purpose of our paper is also to address the coupled diffusion-deformation-fracture problem for an “ideal” single-network polymeric gel. If the cross-linking chemical bonds in such a network are strong then fracture is expected to occur by scission of the chains between the crosslinks, as envisioned in the classical model of Lake and Thomas (1967), while if the chemical crosslinks are weak then fracture is expected to occur because of the scission of the cross-linking bonds themselves. In this paper we focus our attention networks with strong cross-linking bonds which fail by chain-scission.² Further, as in the theory of Broger et al. (2017b), to model the fracture of a gel we introduce a damage variable $d(\mathbf{X}, t) \in [0, 1]$. If $d = 0$ at a point then that point is intact, while if $d = 1$ at some point, then that point is fractured. Values of d between zero and one correspond to partially-fractured material. We assume that d grows monotonically so that $\dot{d}(\mathbf{X}, t) \geq 0$, which is a constraint that represents the usual assumption that microstructural changes leading to fracture are irreversible. As in Broger et al. (2017b) our theory also accounts for the gradient of the damage variable, ∇d . However, in contrast to the particular “incremental variational” approach taken by these authors in formulating their theory, we formulate our gradient-damage theory by using Gurtin’s pioneering virtual-power approach (Gurtin, 1996; 2002). This approach leads to macroforce and microforce balances for the forces associated with the rate-like kinematical descriptors in the theory. These macro- and microforce balances, together with a free-energy imbalance law under isothermal conditions, when supplemented with a set of thermodynamically-consistent constitutive equations, provide the governing equations for our theory. The particular constitutive equations for fracture of a gel in our paper are based on extensions of a physical model of fracture of dry

¹ The origins of the regularization of a sharp crack discontinuity in their diffuse-crack theory may be traced back to the energy minimization concepts of brittle fracture mechanics proposed in Francfort and Marigo (1998) and Bourdin et al. (2000).

² We leave a consideration of interpenetrating-multiple-network gels, as well as materials which exhibit additional non-trivial dissipation mechanisms such as viscoelasticity and Mullins-effect, to future efforts.

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