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A micromechanical damage and fracture model for polymers based on fractional strain-gradient elasticity

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ABSTRACT

We formulate a simple one-parameter macroscopic model of distributed damage and fracture of polymers that is amenable to a straightforward and efficient numerical implementation. We show that the macroscopic model can be rigorously derived, in the sense of *optimal scaling*, from a micromechanical model of chain elasticity and failure regularized by means of *fractional strain-gradient elasticity*. In particular, we derive optimal scaling laws that supply a link between the single parameter of the macroscopic model, namely, the critical energy-release rate of the material, and micromechanical parameters pertaining to the elasticity and strength of the polymer chains and to the strain-gradient elasticity regularization. We show how the critical energy-release rate of specific materials can be determined from test data. Finally, we demonstrate the scope and fidelity of the model by means of an example of application, namely, Taylor-impact experiments of polyurea 1000 rods.

1. Introduction

The use of polymers as structural materials is critically limited by their tendency to degrade by distributed damage or to fail by fracture, sometimes in a brittle manner (cf. e.g., Andrews 1968, Bikales 1971, Kinloch and Young 1983, Williams 1984, Kausch 1985, Grellmann and Seidler 2001, Argon 2013 for reviews). Damage in polymers deformed under tensile loading often takes the form of distributed voids (Jiao et al., 2006, 2007, 2009, Weinberg and Reppel 2014), cf. Fig. 1. Voids nucleate heterogeneously from flaws or inclusions, Fig. 1a, and subsequently grow under tension, Fig. 1b, resulting in softening—or loss of bearing capacity—of the material (cf. e.g., Gent 1973, Cho and Gent 1988, Gent and Wang 1991). Likewise, fracture in polymers can often be traced to the formation of crazes (cf. e.g., Donald and Kramer 1982, Kausch 1983, Henkee and Kramer 1986, Kramer and Berger 1990, Sanderson and Pasch 2004), Fig. 2. Crazes are thin layers of highly localized tensile deformation. The craze surfaces are bridged by numerous fine fibrils, themselves consisting of highly oriented chains, separated by connected voids. Crazes undergo several stages along their formation, including nucleation, growth and final breakdown, resulting in the formation of a traction-free crack, or fracture. Craze initiation is likely the result of heterogeneous cavitation at flaws loaded under conditions of high triaxiality. Craze propagation has been linked to a meniscus instability resulting in the formation of fibrils. This analogy is immediately suggestive of some role played by surface energy

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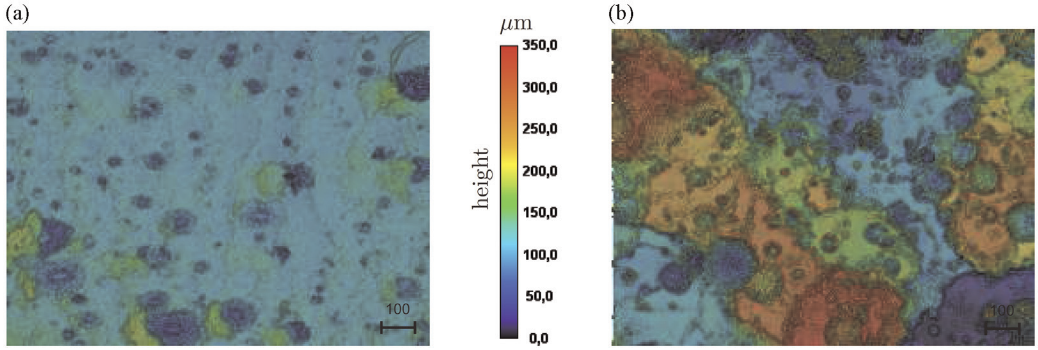

Fig. 1. Surface profiles (height measured from the deepest point) of a polyurea specimen tested in uniaxial tension (Weinberg and Reppel 2014). (a) Initial profile showing initial porosity. (b) Profile after fracture showing proliferation of voids.

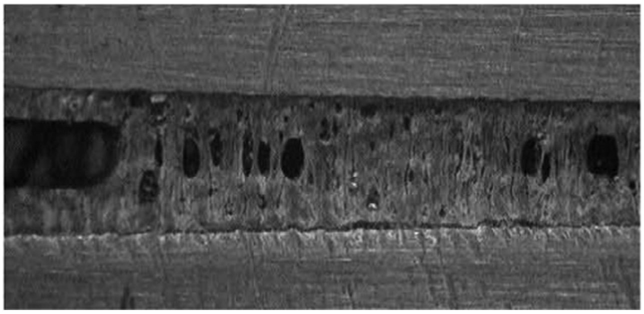

Fig. 2. Crazing process in a steel/polyurea/steel sandwich specimen under opening mode fracture (Zhu et al., 2009).

or other similar physical properties not accounted for by bulk behavior. Eventually, crazes break down to form cracks. Experimentally, crazes are easily identified and observed fractographically by a variety of techniques including optical interferometry, light reflectometry, dark-field electron microscopy, and others.

Owing to its engineering importance, polymer damage and fracture have been the focus of extensive modeling. A number of micromechanical and computational models, ranging from atomistic to continuum, have been put forth (cf. e.g., Leonov and Brown 1991; Krupenkin and Fredrickson 1999a,b; Tijssens et al., 2000a,b; Estevez et al., 2000a,b; Baljon and Robbins 2001, Socrate et al., 2001, Drozdov 2001, Tijssens and van der Giessen 2002, Rottler and Robbins 2003, 2004, Basu and Mahajan 2005, Saad-Gouider et al., 2006, Zairi et al., 2008, Seelig and Van der Giessen 2009, Reina et al., 2013), including consideration of nucleation and growth of voids, craze nucleation, network hardening and disentanglement, chain strength, surface energy and other, that account, to varying degrees, for the observational evidence and relate macroscopic properties to material structure and behavior at the microscale. In parallel a large mathematical literature has evolved, discussing the possibility of cavitation in local models and possible nonlocal extensions which may ensure existence of minimizers, see for example Ball (1982), James and Spector (1991), Müller and Spector (1995), Conti and DeLellis (2003) and Henao and Mora-Corral (2010). These advances notwithstanding, the connection between micromechanical properties and polymer fracture, and specifically any scaling laws thereof, has defied rigorous analytical treatment and characterization. Of special interest is the identification of optimal scaling laws relating the macroscopic behavior to micromechanical and loading parameters. Such optimal scaling laws are established by producing upper and lower bounds of a power-law type with matching exponents for all parameters in both bounds. Optimal scaling methods were pioneered by Kohn and Müller (1992) as part of their seminal work on branched structures in martensite, and have been since successfully applied to a number of related problems, including shape-memory alloys, micromagnetics, crystal plasticity, and others (Kohn and Müller 1992, 1994, Choksi et al., 1999, Conti 2000, Conti and Ortiz 2005).

Fokoua et al. (2014, 2014) have recently applied those analysis tools to ductile fracture of metals. They specifically consider the deformation, ultimately leading to fracture, of a slab of finite thickness subject to monotonically increasing normal opening displacements on its surfaces. In addition, they posit two competing constitutive properties, namely, sublinear energy growth and strain-gradient hardening. Sublinear growth (the energy of linear elasticity exhibits quadratic growth, by way of comparison) is a reflection of the work-hardening characteristics of conventional metallic specimens and gives rise to well-known geometric instabilities such as the necking of bars, sheet necking, strain localization and others (cf. e.g., McClintock and Argon 1966). In metals undergoing ductile fracture this inherently unstable behavior is held in check by a second fundamental property of metals, namely, *strain-gradient hardening* (Fleck and Hutchinson 1993, Fleck et al., 1994, Fleck and Hutchinson 1997, 2001). Under these assumptions, Fokoua et al. (2014, 2014) show, through rigorous