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A nonlocal model of fracture by crazing in polymers

S. Heyden [a,*], S. Conti [b], M. Ortiz [a]

[a] Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA
[b] Institut für Angewandte Mathematik, Universität Bonn, Endenicher Allee 60, 53115 Bonn, Germany

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ABSTRACT

We derive and numerically verify scaling laws for the macroscopic fracture energy of polymers undergoing crazing from a micromechanical model of damage. The model posits a local energy density that generalizes the classical network theory of polymers so as to account for chain failure and a nonlocal regularization based on strain-gradient elasticity. We specifically consider periodic deformations of a slab subject to prescribed opening displacements on its surfaces. Based on the growth properties of the energy densities, scaling relations for the local and nonlocal energies and for the specific fracture energy are derived. We present finite-element calculations that bear out the heuristic scaling relations.

1. Introduction

Fracture of polymers can often be traced to the formation of *crazes* (cf., e. g., Kausch, 1983), Fig. 1, consisting of 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 or other similar physical properties not accounted for by bulk behavior. Eventually, crazes break down to form cracks.

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., Socrate et al., 2001; Basu et al., 2005; Seelig and Van der Giessen, 2009 for a sampling), including consideration of nucleation and growth of voids, craze nucleation, network hardening and disentanglement, chain strength, surface energy and other effects. By contrast, there is a paucity of rigorous analytical results relating micromechanical processes such as crazing and the macroscopic fracture properties of polymers.

Heyden et al. (2015) and Conti and Ortiz (2014) have recently presented a rigorous optimal-scaling study and supporting calculations based on a nonlocal damage model. The model posits that the behavior of polymers has two components, *local* and *nonlocal*. The local behavior is characteristic of large material samples deforming uniformly and it represents the configurational statistics of a polymeric chain network in the thermodynamic limit (cf., e. g., Weiner, 2002; Flory, 1969). Heyden et al. (2015) extend the classical network theory by assuming that the chain bonds have a finite strength. When the strength of the chain is reached, the chain is assumed to fail and to subsequently have no load-bearing capacity. They show that, for large deformations, the deformation–theoretical free energy has *zero growth*, i.e., it is bounded above and below by a constant. For completeness and ease of

* Corresponding author.
E-mail addresses: heyden@caltech.edu (S. Heyden), sergio.conti@uni-bonn.de (S. Conti), ortiz@caltech.edu (M. Ortiz).

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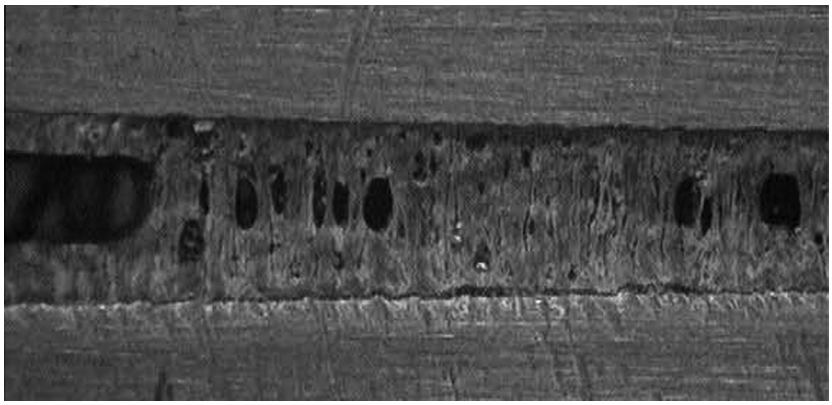

Fig. 1. Crazing process in a steel/polyurea/steel sandwich specimen under opening mode fracture (Zhu et al., 2009).

reference, we briefly summarize the damage model of Heyden et al. (2015) in Section 2.1.

However, energies with sublinear growth relax to zero, i.e., allow the material to fracture with zero expenditure of energy, and thus fail to supply useful information regarding fracture properties. Heyden et al. (2015) assume that, in polymers undergoing fracture, this inherently unstable behavior is stabilized by a second fundamental property, namely *fractional strain-gradient elasticity*, as a generalization of conventional strain-gradient elasticity (cf., e. g., Kröner, 1968; Hermann, 1974; Maugin and Metrikine, 2010) in which the strain-energy density depends on fractional derivatives (cf., e. g., (Adams, 1975)) of the deformation gradient. The need to consider fractional derivatives in the definition of the energy stems from the fact that conventional strain-gradient elasticity is too rigid to enable the type of deformations involved in the crazing mechanism and, hence, is incompatible with experimental observation. The assumption of fractional derivatives removes sufficient rigidity from conventional strain-gradient elasticity to allow for crazing deformations, thus bringing the theory into agreement with experimental observation.

Based on the micromechanical model just described, Heyden et al. (2015) and Conti and Ortiz (2014) derive rigorous optimal scaling laws for the macroscopic fracture energy of polymers. They specifically consider a material sample in the form of an infinite slab of finite thickness subjected to prescribed opening displacements on its two surfaces. For this particular geometry, they derive optimal scaling laws for the dependence of the specific fracture energy on cross-sectional area, micromechanical parameters, opening displacement and intrinsic length of the material. In particular, the upper bound is obtained by means of a construction of the crazing type.

These advances notwithstanding, Conti and Ortiz (2014) point out that a regularization based on conventional strain-gradient elasticity becomes possible if a *core region* is removed along the lines where the deformation second-gradient diverges, namely, the network of lines on the fracture plane from where the connected voids surrounding the fibrils in a craze nucleate. Thus, a local analysis of the deformation in the vicinity of such lines shows that the energy diverges as the radius of the core region, *or core-cutoff radius*, is reduced to zero, cf. Section 2.2. In the particular case in which the nonlocal energy density has linear growth, the energy diverges logarithmically. Thus, the core device is in analogy with the similar device used to eliminate logarithmic energy divergences in the classical theory of linear-elastic dislocations, see for example Hirth and Lothe (1968).

The present work is concerned with the development of scaling laws for the macroscopic fracture energy resulting from a micromechanical model of polymer damage based on strain-gradient elasticity. We specifically consider periodic deformations of a slab subject to prescribed opening displacements on its surfaces. A heuristic derivation of the expected scaling laws is presented in Section 3.1. We argue that, owing to the sublinear growth of the local energy density, the deformation of the slab is localized to a thin layer and that, elsewhere, the slab undergoes a rigid translation through the prescribed opening displacements. The strain-localization layer then further breaks up into periodic cells. Since the deformation is everywhere volume-preserving, the transverse extension of the cells must necessarily result in the formation of cavities. The formation of fibrils results from a process of cavitation from a network of lines contained in the fracture plane. As already noted, this process of cavitation from lines results in infinite energies. We relax this excessive rigidity by assuming a small but finite core around the nucleation lines. Based on the growth properties of the corresponding energy densities, the expected forms of the local and nonlocal energies are set forth in Section 3.1. In particular, the total energy scales with the fracture area, thus resulting in a well-defined specific fracture energy.

One key advantage of the core-cutoff model considered in the present work is that it is readily amenable to a straightforward finite-element implementation, Section 3.2. We use such implementation as a basis for verifying the heuristic scaling relations just described. In particular, the deformation of a unit cell containing a small nucleation borehole is calculated under increasing prescribed opening displacements. The calculations are found to bear out the heuristic scaling relations set forth for the local and nonlocal energies as well as for the specific fracture energy.