A Loading History Agnostic Free Energy Based Fracture Criterion

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Abstract

Rather than energy release rate, the proposed framework starts from the energy function itself. Instead of strain energy density, it considers the change in volume-specific free energy density from mechanical deformation. The free energy function must capture strain induced orthotropy, known to be critical for polymers but also important for metals plasticity. To capture strain induced orthotropy, free energy is defined in terms of principal strains and by separating deformation into dilatational and distortional contributions. The separation does not utilize deviatoric strain. Rather, it leverages a new distortional strain definition and the new concept of orthotropic dilataion, enabling clean separation to large strain.

The proposed framework clarifies how a generalized Maxwell model spring-dashpot mechanical analog cleanly interperets the First and Second Laws of Thermodynamics. A transition state theory based nonlinear viscoelastic (NLVE) model is mated to the Maxwell model. Nonlinear Maxwell springs feature an instability in their constitutive law, providing a viscoelastic failure criterion. Embedding the instability into the springs in an NLVE model provides a failure criterion that accommodates complex temperature histories, rate dependence, and self generated heat from cyclic loading..

1. Mechanics Theory

The change in volume specific free energy from mechanical deformation (Δf) defines principal stress (σ_i):

$$\sigma_i = \frac{\partial \Delta f}{\partial \varepsilon_i} \quad (1)$$

where ε_i are the logarithmic strains in the 3 principal directions. The free energy function is split into distortional and dilatational contributions. A new definition of distortional strains (γ_i) is presented in terms of principal logarithmic strains, ε_i:

$$\gamma_i \equiv \varepsilon_{i+1} - \varepsilon_{i+1} \ , \quad i = 1{,}2{,}3{,}1{,}2 \quad (2)$$

The letter gamma is used, because this distortional strain is equivalent to pure shear at small strains. For the general case of nonlinear orthotropic elasticity, the total distortional contribution to free energy, Δf_s , is:

$$\Delta f_s = \Delta f_1(\gamma_1) + \Delta f_2(\gamma_2) + \Delta f_3(\gamma_3) \quad (4)$$

where $\Delta f_i(\gamma_i)$ are the independent contributions to distortional free energy change from each of the 3 newly defined distortional strains. For initially isotropic materials, these are the same function. Each free energy sub-function is completely defined by its respective strain. The shape of the distortrional free energy function is inspired by Materials Science. For example, wone could use a Gent Hyperelastic model. An added contribution from this effort is including failure in the hyperelasticity by including an instability in the stress-strain response.

The distortional contributions to free energy provided three additional mathematical relationships needed to capture stain induced orthotropy. The shear stresses τ_i are defined as the derivative of the new shear strains:

$$\tau_i \equiv \frac{\partial \Delta f_i}{\partial \gamma_i} \, ; \quad i = 1,2,3 \tag{5}$$

An innovative bulk free energy definition provides the final 3 mathematical relationships needed for orthotropy. The concept of orthotropic dilatation proposes three unique z-functions to describe the dilatational contribution to free energy:

$$\Delta f_b = \frac{1}{2} \{ z_1(\varepsilon_1) + z_2(\varepsilon_2) + z_3(\varepsilon_3) \}^2 \tag{7}$$

The three z-functions of Eq.6 are the key to determining the bulk contribution to strain energy density. The shape of these strain dependent functions is inspired by strain energy density or potential energy functions in Materials Science, such as the Lennard-Jones potential. The dilatational contribution to stress in the three principal directions will be defined as ζ_i :

$$\zeta_i \equiv \frac{\partial \Delta f_b}{\partial \varepsilon_i}; \quad i = 1,2,3 \tag{8}$$

Implementing the chain rule, and combining Equations 1, 5, 8, and 9:

$$\begin{aligned} \sigma_1 &= \frac{2}{3} \, (\tau_3 - \tau_2) \, + \, \zeta_1 \\ \sigma_2 &= \frac{2}{3} \, (\tau_1 - \tau_3) \, + \, \zeta_2 \\ \sigma_3 &= \frac{2}{3} \, (\tau_2 - \tau_1) \, + \, \zeta_3 \end{aligned} \tag{10}$$

Eq.10 shows a clear separation between distortion and dilatation, even for orthotropy. It is also valid to large strains.

2. Conclusions

A mechanics framework has been introduced to capture strain induced orthotropy. The free energy function is defined in terms of principal strains and six separate stress-strain relationships: 3 distortional and 3 dilatational. To capture time and temperature dependence, each of the 6 stress-strain relationships is represented by a generalized Maxwell model. Nonlinear Maxwell springs include an instability. Fracture occurs either in distortion (ie, slip on some length scale), or dilatation (ie, cavitation on some length scale). Embedding the failure criterion in an NLVE model makes it sufficiently robust to predict any loading frequency or any combination of loading frequencies. It also accommodates any contribution from creep during fatigue loading as well as temperature history.