On Irreversibility and Dissipation in Hyperelasticity With Softening

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Bulk and interface material failures are often modeled via hyperelastic stored energy functions incorporating softening behavior. The softening is reversible due to the hyperelastic nature of the constitutive law and material can "heal" under unloading. To prevent this healing, special numerical procedures (like finite element deletion) are usually used in computer simulations. In the present work, we suggest an alternative: very simple analytical formulation, which makes failure irreversible when a critical stored energy is reached. This new notion is directly incorporated into the constitutive equations, consequently, relieving the need for preliminary discretization of the boundary-value problem.
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1 Introduction

Continuum mechanics approaches to modeling material failure can be provisionally divided into two groups: surface and bulk models. Neither is overall superior, and each method is preferable for different problems.

Surface or interface failure models appear by the name cohesive zone models (CZMs) in the modern literature. A cohesive zone is a surface in bulk material where displacement discontinuities occur. Thus, continuum is enhanced with discontinuities, which require additional traction-separation constitutive equations. The latter equations are constructed qualitatively as follows: traction increases, reaches a maximum, and then tends to zero with increasing separation. Cohesive zones can be inside finite elements (XFEM) or along their boundaries. Hyperelastic constitutive descriptions of traction-separation were used in the pioneering finite element simulations by Needleman [1] and Xu and Needleman [2,3]. Sophisticated modern versions of hyperelastic CZMs can be found in Ref. [4], for example.

Bulk failure models appear by the name continuum damage mechanics (CDM) in the modern literature. In CDM, material failure or damage is modeled by constitutive equations incorporating softening, i.e., descending stress-strain curves. For example, physically appealing continuum-atomistic methods [5–7] use empirical potentials, which include a possibility of full molecular separation. These models are hyperelastic. Another simple approach to modeling bulk failure was proposed by Volokh [8–11] in which no phenomenological atomistic potentials were involved and the energy, which could be stored and dissipated by infinitesimal material volume, was limited.

Though simple and mimicking molecular interactions, hyperelastic (surface and bulk) models have a drawback—they can lead to material healing and restoration of dissipated energy under unloading. At the molecular or atomistic level, the healing effect might be natural, but normally it is not reproduced at the macroscopic level. Macroscopically, molecules and atoms at the surface of cracks undergo significant rearrangement, and cracks do not disappear after unloading.

To prevent material healing within hyperelastic frameworks, special numerical procedures are often employed in simulations. For instance, it is possible to delete finite elements where the material has failed. Actually, the element deletion is a general computational approach to handle material failure, and it is used in inelastic material models as well. Although the element deletion procedure (as well as other numerical approaches) is practical, a model which inherently accounts for irreversibility is desired, namely, one which resolves dissipation issues on the analytic level of constitutive equations prior to any spatial discretization.

In Secs. 2 and 4, we suggest a very simple analytical formulation, which furnishes a failure description irreversible when critical storage energy is reached. As mentioned above, this new formulation is incorporated in the constitutive equations directly, consequently, relieving the need for any preliminary discretization of the boundary-value problem. We use the boundary value problem of uniaxial tension of natural rubber in Sec. 3 to illustrate the new constitutive formulation. Although the proposed technique is similarly applicable to hyperelastic cohesive zone models, we restrict our considerations to bulk hyperelasticity with softening.

Remark 1. The problem of healing is not just a question of unloading but also a question of time scale. Open cracks may heal with time due to various physical and chemical effects. Numerous examples exist for time dependent healing in biological and geological materials. We emphasize the absence of immediate healing upon unloading as the objective of this work.

Remark 2. We restrict our attention to elastic material behavior. The progress in inelastic failure simulations, especially for cohesive-zone models, can be found for instance in Refs. [12–16].

2 Governing Equations

The stored energy function for hyperelastic material with softening can be written in the following general form [8,9]:

$$\psi = \psi^{\text{failure}} - \psi^{\text{elastic}}(\mathbf{C}) \tag{1}$$

where $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is the right Cauchy–Green tensor; $\mathbf{F} = \partial\mathbf{y}(\mathbf{x})/\partial\mathbf{x}$ is the deformation gradient for material point $\mathbf{x}$ that moves to position $\mathbf{y}(\mathbf{x})$ in the current configuration of body Ω.

Terms on the right side of Eq. (1) have the following properties:

$$\psi^{\text{failure}} = \psi^{\text{elastic}}(\mathbf{1}) \tag{2}$$

$$\psi^{\text{elastic}}(\mathbf{C}) \to 0, \quad \text{when } \|\mathbf{C}\| \to \infty \tag{3}$$

where $\mathbf{1}$ is a second-order identity tensor and $\|\mathbf{C}\| = \mathbf{C} : \mathbf{C} = \text{tr}\mathbf{C}^2$, for example

Thus, ψ^{failure} and $\psi^{\text{elastic}}(\mathbf{C})$, respectively, designate constant bulk failure energy and an elastic energy.

Hyperelastic material—described above—returns to its initial state under unloading. To prevent this healing, we modify the stored energy function as follows:

$$\psi = \psi^{\text{failure}} - H(\alpha)\psi^{\text{elastic}}(\mathbf{C}) \tag{4}$$

$$\dot{\alpha} = -H\left(\varepsilon - \frac{\psi^{\text{elastic}}}{\psi^{\text{failure}}}\right), \quad \alpha(t=0) = 0 \tag{5}$$

$$H(z) = \begin{cases} 0, & z < 0 \\ 1, & z \geq 0 \end{cases} \tag{6}$$

where $0 < \varepsilon \ll 1$ is a dimensionless precision constant, and $H(z)$is a unit step function.

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The physical interpretation of Eqs. (4)–(6) is simple: Material response is hyperelastic as long as the stored energy is below its limit ψ^{failure}. When the limit is reached, the stored energy remains constant for the rest of the deformation process, thereby, making material healing impossible. The parameter $\alpha \in (-\infty, 0]$ functions as a *switch*: If $\alpha = 0$ the process is hyperelastic and reversible, and if $\alpha < 0$ the material is irreversibly damaged and the stored energy is dissipated.

Constitutive equations can be derived from Eq. (4) via a thermodynamic argument. Let us consider the dissipation inequality

$$\frac{1}{2}\mathbf{S} : \dot{\mathbf{C}} - \dot{\psi} \geq 0 \tag{7}$$

where $\mathbf{S}$ is the second Piola–Kirchhoff stress tensor.

The energy increment is calculated from Eqs. (4)–(6) as follows:

$$\dot{\psi} = -\delta(\alpha)\dot{\alpha}\psi^{\text{elastic}} - H(\alpha)\frac{\partial \psi^{\text{elastic}}}{\partial \mathbf{C}} : \dot{\mathbf{C}} \tag{8}$$

where $\delta(\alpha)$ is the Dirac δ.

Substituting Eq. (8) in Eq. (7) yields

$$\left(\frac{1}{2}\mathbf{S} + H(\alpha)\frac{\partial \psi^{\text{elastic}}}{\partial \mathbf{C}}\right) : \dot{\mathbf{C}} + \delta(\alpha)\dot{\alpha}\psi^{\text{elastic}} \geq 0 \tag{9}$$

We notice that the second term on the LHS of Eq. (9) in fact vanishes for all values of α. The case of $\alpha \neq 0$ follows immediately from the definition of Dirac's δ. In the case of $\alpha = 0$, we note that the relation $\alpha = \int \dot{\alpha} dt = 0$ along with the definition of $\dot{\alpha}$ as a step function imply $\dot{\alpha} \equiv 0$ since a nonpositive integrand must be identically zero for the integral to vanish.

Thus, the dissipation inequality is obeyed by setting the constitutive law in the form

$$\mathbf{S} = -2H(\alpha)\frac{\partial \psi^{\text{elastic}}}{\partial \mathbf{C}} \tag{10}$$

To complete the boundary-value problem, we set the balance of linear momentum (without body and inertia forces) inside the body Ω as follows:

$$\text{Div}(\mathbf{FS}) = \mathbf{0} \tag{11}$$

where the divergence operator is applied with respect to referential coordinates $\mathbf{x}$.

Balance of linear momentum on the body surface $\partial\Omega$ reads

$$\mathbf{FSn} = \bar{\mathbf{T}} \tag{12}$$

where $\bar{\mathbf{T}}$ is a prescribed traction per unit area of the reference surface with the unit outward normal $\mathbf{n}$.

Alternatively to Eq. (12), boundary conditions can be imposed upon placements

$$\mathbf{y} = \bar{\mathbf{y}} \tag{13}$$

where the barred quantity is prescribed on the surface $\partial\Omega$.

3 Uniaxial Tension and Failure of Natural Rubber

In this section, we solve the governing equations set above in the case of uniaxial tension of natural rubber.

Following Ref. [10], we define the elastic energy as

$$\psi^{\text{elastic}} = \frac{\Phi}{10}\Gamma\left(\frac{1}{10}, \frac{W^{10}}{\Phi^{10}}\right) \tag{14}$$

$$W = C_1(I_1 - 3) + C_2(I_1 - 3)^2 + C_3(I_1 - 3)^3, \quad I_1 = \text{tr}\mathbf{C}, \quad \det \mathbf{F} = 1 \tag{15}$$

$$C_1 = 0.298\,\text{MPa}, \quad C_2 = 0.014\,\text{MPa}, \quad C_3 = 0.00016\,\text{MPa}, \quad \Phi = 82.0\text{MPa} \tag{16}$$

where $\Gamma(s, x) = \int_x^\infty t^{s-1}\exp(-t)dt$ is the upper incomplete γ function; $W(\mathbf{C})$ is the stored energy of intact (without failure) material; and Φ is the energy limiter, which was calibrated in macroscopic experiments.

For uniaxial tension we have

$$\mathbf{F} = \lambda \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda^{-1/2}\mathbf{e}_2 \otimes \mathbf{e}_2 + \lambda^{-1/2}\mathbf{e}_3 \otimes \mathbf{e}_3 \tag{17}$$

$$\mathbf{S} = S\mathbf{e}_1 \otimes \mathbf{e}_1 \tag{18}$$

$$S = 2H(\alpha)(1 - \lambda^{-3})W_1 \exp(-W^{10}/\Phi^{10}) \tag{19}$$

$$W_1 \equiv \partial W/\partial I_1 = C_1 + 2C_2(I_1 - 3) + 3C_3(I_1 - 3)^2 \tag{20}$$

$$I_1 = 2\lambda^{-1} + \lambda^2 \tag{21}$$

where λ is the principal stretch along direction of tension x_1.

Since stress and deformation are homogeneous, equilibrium Eq. (11) is obeyed identically and traction is obtainable from Eqs. (12) and (17)–(20), given by $\bar{T}_1 = \lambda S$.

It is convenient to present the stress-stretch curve in terms of the true (Cauchy) stress

$$\boldsymbol{\sigma} = (\det \mathbf{F})^{-1}\mathbf{FSF}^T = \sigma \mathbf{e}_1 \otimes \mathbf{e}_1 \tag{22}$$

$$\sigma = 2H(\alpha)(\lambda^2 - \lambda^{-1})W_1 \exp(-W^{10}/\Phi^{10}) \tag{23}$$

Let us assume that stretching is performed monotonically at a constant rate

$$\lambda = \dot{\lambda}t + 1, \quad \dot{\lambda} = \text{constant}, \quad t \in [0, \infty) \tag{24}$$

Then, we can integrate Eq. (5) as follows:

$$\alpha\dot{\lambda} = -H\left(\varepsilon - \frac{\psi^{\text{elastic}}}{\psi^{\text{failure}}}\right)(\lambda - \lambda_0) \tag{25}$$

where λ_0 is a solution of equation $\varepsilon\psi^{\text{failure}} = \psi^{\text{elastic}}$.

Graphs defined by Eqs. (23) and (25) are presented in Fig. 1 for $\varepsilon = 0.0001$.

Stars designate the point where failure and dissipation become irreversible. Smaller precision constant ε will not affect results. Larger ε may lead to earlier irreversible failure.

4 Generalization

The formulation presented above is useful in the case of isotropy. When material response is anisotropic [17], it might be necessary to split the energy function into a sum as follows:

$$\psi = \sum_{n=1}^{N} \psi_n \tag{26}$$

$$\psi_n = \psi_n^{\text{failure}} - H(\alpha_n)\psi_n^{\text{elastic}}(\mathbf{C}) \tag{27}$$

$$\dot{\alpha}_n = -H\left(\varepsilon_n - \frac{\psi_n^{\text{elastic}}}{\psi_n^{\text{failure}}}\right), \quad \alpha_n(t = 0) = 0 \tag{28}$$

where the nth component represents a constituent or characteristic direction.

We note that according to Eqs. (26)–(28) failure of the nth constituent does not lead to overall failure.

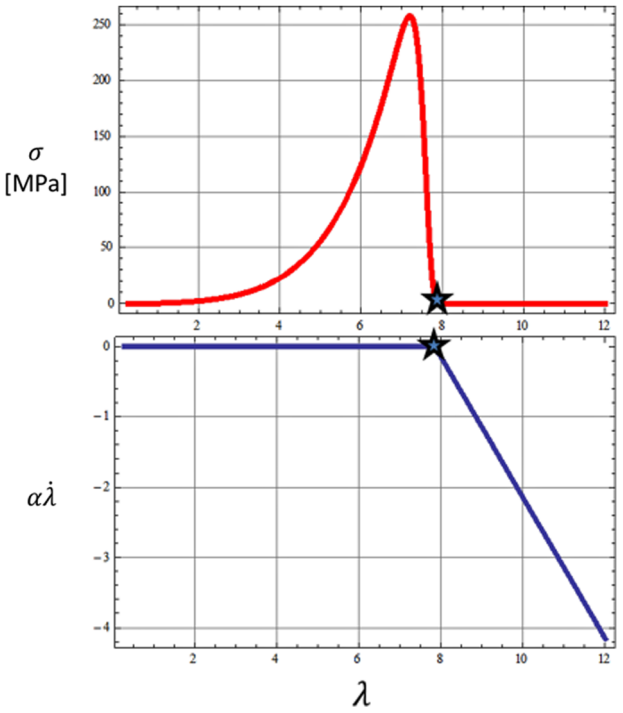

Fig. 1 Cauchy stress and switch parameter versus stretch in uniaxial tension

It is possible to modify the formulation in such a way that failure of any constituent will lead to overall failure. This can be achieved, for instance, as follows:

$$\psi = \sum_{n=1}^{N} \beta_n \psi_n \tag{29}$$

where

$$\beta_n = \prod_{\substack{j=1 \\ j \neq n}}^{N} H(\alpha_j) \tag{30}$$

For example, in the case of $N = 2$ we have

$$\begin{aligned} \psi = {} & H(\alpha_2)(\psi_1^{\text{failure}} - H(\alpha_1)\psi_1^{\text{elastic}}(\mathbf{C})) \\ & + H(\alpha_1)(\psi_2^{\text{failure}} - H(\alpha_2)\psi_2^{\text{elastic}}(\mathbf{C})) \end{aligned} \tag{31}$$

This two-component case can be relevant for the transversely isotropic bulk material or CZM where different failure descriptions are used for tangent and normal tractions.

Finally, we can derive the corresponding constitutive equation by using the thermodynamic argument as in Sec. 2. Omitting intermediate manipulations, we get

$$\mathbf{S} = -2 \prod_{j=1}^{N} H(\alpha_j) \sum_{n=1}^{N} \frac{\partial \psi_n^{\text{elastic}}}{\partial \mathbf{C}} \tag{32}$$

5 Conclusion

We presented a new constitutive formulation for hyperelasticity with softening that enforced irreversibility and dissipation in failure description. This formulation is very simple, and it can be easily implemented in computer simulations. Although only bulk failure was addressed in the present work, the described approach can be effortlessly adapted to hyperelastic cohesive-zone models as well. Finally, we note that only a formal description of irreversibility and dissipation within the framework of hyperelasticity with softening has been addressed in the present work. Mesh-dependency issues and regularization strategies will be considered separately elsewhere.

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