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A computational framework for gradient-enhanced damage – implementation and applications

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A gradient-enhanced damage model is combined with finite viscoelasticity and implemented in an Abaqus user subroutine, exploiting the heat equation solution capabilities for the damage regularisation, in order to simulate soft polymers. This regularised damage approach provides the advantage of mesh independent results and avoids localisation effects. In this work, a self-diagnostic poly(dimethylsiloxane) (PDMS) elastomer is chosen as an example. To this end, an efficient two-step parameter identification framework is developed to calibrate the corresponding model parameters.

1 Introduction

Nowadays, the applications of lightweight components in industrial products vastly increases. Consequently, the mass reduction, while still maintaining the required mechanical properties, e.g. stiffness or notched bar impact strength, is of high importance. In addition, in many forming processes or loading cases of the components, the damage initiation starts due to pore growth. As a result, the material properties change in an uncontrolled manner. Hence, more accurate damage models, especially those avoiding localisation effects, are required, e.g. the used gradient-enhanced damage model, cf. [1]. For further applications of the damage model, e.g in combination with finite plasticity, see [2]. Apart form the model development, the calibration of these complex material models is important. In this work, the damage model is applied to finite viscoelasticity, implemented in an Abaqus UMAT user subroutine and a parameter identification framework was developed in order to properly calibrate the model parameters. Finally, exemplary results are presented to demonstrate the mesh independence.

2 Gradient-enhanced damage – application to finite viscoelasticity

In order to gain mesh independent results, a variationally consistent gradient-enhanced damage regularisation method presented by *Ostwald et al.* [1] is used. Therefore the local Helmholtz free energy potential is extended with two additional non-local terms, such that the total potential takes the form $\psi = \psi_{\rm loc} + \psi_{\rm nloc}$. While the first term of the non-local contribution contains the gradient of the non-local damage variable ϕ and is controlled by the regularisation parameter $c_{\rm d}$, the second term penalises the deviation between ϕ the non-local and κ the local damage variable with the penalty parameter $\beta_{\rm d}$, so that

$$\psi_{\rm nloc}(\boldsymbol{F}, \phi, \nabla_{\boldsymbol{X}}\phi, \kappa) = \tfrac{1}{2}\, c_{\rm d}\, \nabla_{\boldsymbol{x}}\phi \cdot \nabla_{\boldsymbol{x}}\phi + \tfrac{1}{2}\, \beta_{\rm d}\, [\, \phi - \kappa\,]^2 \,. \tag{1}$$

Following the postulate of maximum dissipation, the evolution equation of the internal damage variable takes the form

$$\dot{\kappa} = \lambda\, \partial_q \Phi_{\rm d}(\boldsymbol{F}, \phi, \nabla_{\boldsymbol{X}}\phi, \kappa)\,, \tag{2}$$

with λ denoting the Lagrange multiplier, $\Phi_{\rm d}$ the damage condition and $q = -\partial_d\, \psi$ representing the energy release rate. Consequently, the balance of linear momentum and the Euler-Lagrange equation for the non-local damage field have to be solved simultaneously. Since the Euler-Lagrange equation governing the non-local damage variable is comparable to the heat equation, this approach was implemented in an Abaqus user material subroutine (UMAT) by exploiting the solution capabilities of the heat equation in Abaqus. This technique avoids the necessity of an implementation as a user element subroutine (UEL) including the difficulties of postprocessing or combination with contact mechanics. An exponential format is chosen for the damage function incorporating a damage initiation threshold $\kappa_{\rm d}$, i.e., $f_{\rm d}(\kappa) = 1 - d = \exp(-\eta_{\rm d}\langle \kappa - \kappa_{\rm d}\rangle)$, where $f_{\rm d} \in (0, 1]$ and $\eta_{\rm d}$ denotes the exponential damage saturation rate. In addition, a volumetric-isochoric split of the local energy contribution is introduced in order to model the initiation of damage of both terms with different intensities

$$\psi_{\rm loc}(\boldsymbol{C}, \kappa) = f_{\rm d}(\kappa)\, \psi_{\rm vol}(J) + f_{\rm d}^{n_{\rm iso}}(\kappa)\, \psi_{\rm ich}(\bar{\boldsymbol{C}})\,, \tag{3}$$

where $n_{\rm iso}$ controls the isochoric damage contribution and $\bar{\boldsymbol{C}} := J^{-2/3}\boldsymbol{C}$, with $\boldsymbol{C} = \boldsymbol{F}^{\rm t} \cdot \boldsymbol{F}$ and $J = \det(\boldsymbol{F})$.

In this work, the gradient-enhanced damage framework is applied to a rate-dependent finite viscoelasticity model in order to model the damage evolution in polymers. In this case, as an example, a self-diagnostic poly(dimethylsiloxane) (PDMS)

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elastomer, generating a chemical response towards mechanical loads, developed by *Früh et al.* [3], was selected. To this purpose, considering the material behaviour, the Yeoh energy potential, see [4], is chosen for the isochoric energy contribution ψ_{ich} while the volumetric part ψ_{vol} follows a standard fashion, so that

$$\psi_{\text{ich}} = \sum_{i=1}^{3} C_i \left[\text{tr}(\bar{\boldsymbol{C}}) - 3 \right]^i \quad \text{and} \quad \psi_{\text{vol}} = \tfrac{1}{2} K \left[\tfrac{1}{2} \left[J^2 - 1 \right] - \ln(J) \right] , \tag{4}$$

where K denotes the bulk modulus and C_i represent further material parameters. The viscoelastic model follows [5], such that a finite strain generalisation of a classic generalised relaxation model with two Maxwell elements is considered. The evolution of the stress-type internal variables – including relaxation time parameters τ_i and relative moduli γ_i – is given by

$$\dot{\boldsymbol{Q}}_i(t) + \frac{1}{\tau_i} \boldsymbol{Q}_i(t) = \frac{\gamma_i}{\tau_i} \text{DEV}\big(2\, \partial_{\bar{\boldsymbol{C}}} \psi_{\text{ich}}(\bar{\boldsymbol{C}}(t))\big) \quad \text{with} \quad \lim_{t \to -\infty} \boldsymbol{Q}_i(t) = \boldsymbol{0} . \tag{5}$$

3 Calibration of the model and mesh-objective results

Considering the large amount of material parameters, a two-step parameter identification framework was implemented. At first, the Yeoh parameters C_i and the relaxation parameters were calibrated with respect to experiments inducing homogeneous deformation states. Hence, apart from tensile tests, relaxation and creep tests were conducted. In the second step, the already identified subset of parameters is fixed for the identification of the damage related material parameters comparing the simulated material response with experimental data from a tensile test incorporating inhomogeneous deformation states. Characteristic time steps of the experiment with a notched specimen are shown in Figure 1. Figure 2 a) presents the comparison of the experimentally measured load-displacement-curve with the simulated responses for the initial guess of the damage-related material parameters as well as the optimised set including two different mesh discretisations. The load-displacement-curves in combination with the contour plots of the damage value for both mesh discretisations demonstrate mesh-objective results. For further details, see [6].

Fig. 1: Photos of the tensile test with inhomogeneous deformation states of a notched specimen **a)** at the beginning of the experiment at $t = 2.55\,\text{s}$ and **b)** before the sample starts to tear at $t = 1139.8\,\text{s}$; cf. [6].

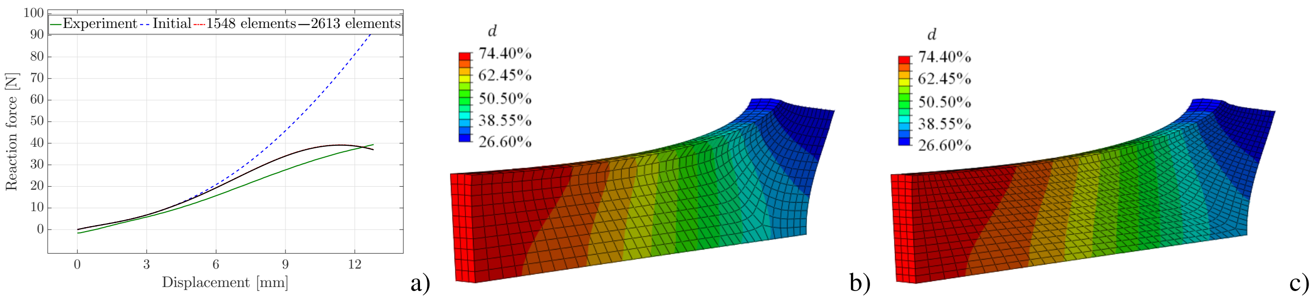

Fig. 2: **a)** Load-displacement curves of the tensile test with the notched specimen reflecting experimental response before rupture and the simulated results for the initial guess of the identification and the optimised set with two different meshes. **b)** Distributon of the damage value of the notched specimen using symmetry properties for a mesh distribution of 1548 and **c)** 2613 elements.

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