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Continuum mechanical modeling of processing induced initial anisotropy in the finite strain deformation of amorphous thermoplastic polymers

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Summary: This work deals with modeling the mechanical behavior of thermoplastic polymers in the finite strain regime over a wide range of temperatures. Thereby, special emphasis is put on the incorporation of an initial anisotropy in terms of "frozen-in" molecular orientation which results from a preceding manufacturing process. A computational example is discussed which considers an injection molded plate undergoing inhomogeneous deformation (buckling) during re-heating.

Introduction

Manufacturing processes of amorphous thermoplastic polymers at elevated temperatures (e.g. injection molding) and subsequent rapid cooling result in an anisotropic microstructure due to "frozen-in" molecular orientation [5]. This state of pre-orientation in the solid material affects the subsequent finite strain deformation behavior in terms flow strength and hardening and may give rise to stress-free deformations of a component during re-heating.
This "memory-effect" can be observed at the injection molded plate in Fig. 1a. After uniformly heating the plate above the glass transition temperature it deforms and buckles due to the pre-oriented microstructure (Fig. 1c). To get some indication of the microstructure one can use polarized light to visualize (via birefringence) regions with high molecular orientation and residual stress (Fig. 1b).

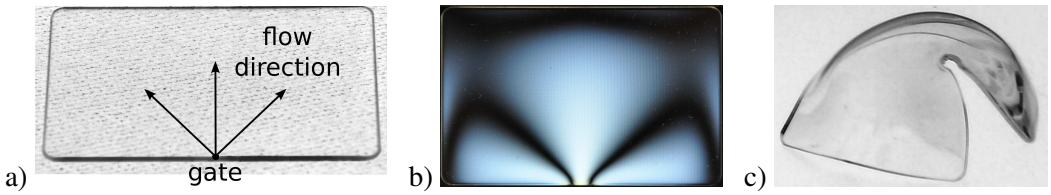

Figure 1: a) Injection molded plate, b) plate under polarized light, c) deformed plate after re-heating above glass transition temperature

The aim of this work is to model the mechanical behavior of thermoplastic polymers in the finite strain regime over a wide range of temperatures (above glass transition) with consideration of a processing induced initial anisotropy. Therefore, experimental test data at different temperatures and strain rates are necessary in order to describe the stress-strain response correctly. Uniaxial tension tests on PMMA at different strain rates and temperatures (below and above glass transition which for PMMA is $T_g \approx 105°$ C) were performed. These tension tests were evaluated using digital image correlation [4] which allows to measure local strain fields needed to determine the

true stress-strain response of the material (Fig. 2). At moderate temperatures the material shows a glassy behavior with an elastic regime followed by inelastic deformation including progressive hardening. At higher temperatures, near to or above the glass transition, the material is in the rubbery state. Elastic strains then are much larger and the separation of elastic and inelastic deformation is less obvious. Furthermore, a rate dependency is observed which is more pronounced at high temperatures so that the glass transition is not a fixed temperature but is rate dependent as well.

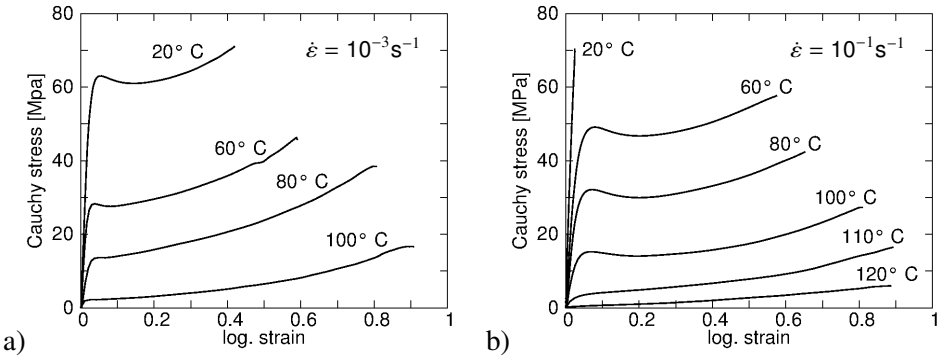

Figure 2: Uniaxial tension tests at different temperatures and strain rates: a) $\dot{\varepsilon} = 10^{-3}s^{-1}$, b) $\dot{\varepsilon} = 10^{-1}s^{-1}$

Continuum mechanical modeling

The material model presented here is based on that developed by Boyce and co-workers [1-3]. Starting with the kinematics, the widely used multiplicative split of the deformation gradient into an elastic and plastic part is utilized

$$\boldsymbol{F} = \boldsymbol{F}^e \boldsymbol{F}^p \tag{1}$$

where $\boldsymbol{F}^p$ defines the stress free configuration after elastic unloading (referred to as the intermediate configuration). Physically, $\boldsymbol{F}^p$ describes permanent molecular orientation in the material. In order to include an initial anisotropy, the inelastic deformation gradient is complemented by an initial deformation gradient $\boldsymbol{F}^i$ (= $\boldsymbol{V}^i$) so that the network deformation tensor $\boldsymbol{F}^n$ is defined as [2]

$$\boldsymbol{F}^n = \boldsymbol{F}^p \boldsymbol{F}^i \ . \tag{2}$$

This network deformation tensor is used in the following to describe the entropic resistance of the molecular network against plastic flow (see below).

The split of the deformation gradient (1) leads to an additive decomposition of the velocity gradient tensor into an elastic and plastic part $\boldsymbol{L} = \boldsymbol{L}^e + \boldsymbol{L}^p$ with the inelastic velocity gradient in the current configuration $\boldsymbol{L}^p = \boldsymbol{F}^e \hat{\boldsymbol{L}}^p \boldsymbol{F}^{e-1}$ and in the intermediate configuration $\hat{\boldsymbol{L}}^p = \dot{\boldsymbol{F}}^p \boldsymbol{F}^{p-1}$. The latter can be decomposed as $\hat{\boldsymbol{L}}^p = \hat{\boldsymbol{D}}^p + \hat{\boldsymbol{W}}^p$ with the inelastic rate of deformation tensor $\hat{\boldsymbol{D}}^p$ and the inelastic spin tensor $\hat{\boldsymbol{W}}^p$, both in the intermediate configuration. While $\hat{\boldsymbol{D}}^p$ is constitutively prescribed via a flow rule, the inelastic spin tensor can be computed as $\hat{\boldsymbol{W}}^p = \boldsymbol{W} - \overset{\curvearrowright}{\boldsymbol{W}}[\boldsymbol{D} + \hat{\boldsymbol{D}}^p]$ with the forth order tensor $\overset{\curvearrowright}{\boldsymbol{W}}$ once the assumption of a symmetric elastic deformation gradient $\boldsymbol{F}^{eT} = \boldsymbol{F}^e$ is made [3].

The inelastic part of the rate of deformation tensor $\hat{\boldsymbol{D}}^p$ in the intermediate configuration is determined by the deviatoric part of the driving stress tensor $\hat{\boldsymbol{\Sigma}} - \hat{\boldsymbol{b}}$ and the plastic shear strain rate $\dot{\gamma}^p$

according to

$$\hat{\boldsymbol{D}}^p = \dot{\gamma}^p \frac{\hat{\boldsymbol{\Sigma}}' - \hat{\boldsymbol{b}}'}{|\hat{\boldsymbol{\Sigma}}' - \hat{\boldsymbol{b}}'|} \qquad , \qquad \dot{\gamma}^p = \dot{\gamma}_0^p \exp\left[-\frac{As}{T}\left(1 - \left(\frac{|\hat{\boldsymbol{\Sigma}}' - \hat{\boldsymbol{b}}'|}{s}\right)^{\frac{5}{6}}\right)\right] \tag{3}$$

with material parameters A, s, $\dot{\gamma}_0^p$ and the temperature T.
The driving stress $\hat{\boldsymbol{\Sigma}} - \hat{\boldsymbol{b}}$ is the difference of the Mandel stress $\hat{\boldsymbol{\Sigma}} = \det(\boldsymbol{F})\boldsymbol{F}^e\boldsymbol{\sigma}\boldsymbol{F}^{e-1}$ (with $\boldsymbol{\sigma}$ being the Cauchy stress tensor) and the backstress $\hat{\boldsymbol{b}}$ (Fig. 3a). The backstress tensor is determined from the Arruda-Boyce eight-chain-model [1]

$$\hat{\boldsymbol{b}} = \frac{C^R\sqrt{N}}{3\lambda_c}\mathcal{L}^{-1}\left(\frac{\lambda_c}{\sqrt{N}}\right)\hat{\boldsymbol{B}}^n \tag{4}$$

with the left Cauchy-Green tensor $\hat{\boldsymbol{B}}^n = \boldsymbol{F}^n\boldsymbol{F}^{nT}$, the inverse of the Langevin-function $\mathcal{L}$, the rubbery modulus C^R, the average number N of rigid links between entanglements and the mean chain stretch $\lambda_c = \left(\frac{1}{3}\mathrm{tr}\hat{\boldsymbol{B}}^n\right)^{\frac{1}{2}}$. In (4) use is made of the network deformation gradient tensor $\boldsymbol{F}^n$ (2) so that an initial backstress can be prescribed. The Cauchy stress $\boldsymbol{\sigma}$ depends on the elastic left Cauchy-Green tensor $\boldsymbol{B}^e = \boldsymbol{F}^e\boldsymbol{F}^{eT}$ and is determined from a hyperelastic Neo-Hooke model. In addition, the model is modified to capture a wide range of temperatures. Therefore, the shear modulus, the material parameter A in (3) and the molecular network parameter N are taken temperature dependent as suggested in [1]. In Fig. 3b the stress-strain response of the model is shown in comparison with experimental data.

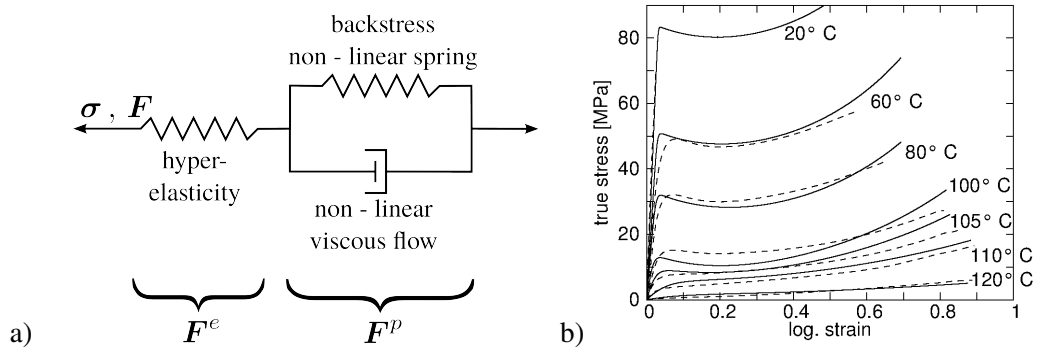

Figure 3: a) Rheological model, b) stress-strain response of the model (dashed lines) and experimental data (solid lines) for a strain rate of $\dot{\varepsilon} = 0.1s^{-1}$

Computational example

As a computational example the injection molded plate shown in Fig. 1a is investigated. An indication of the "frozen-in" molecular orientation (and stretch) is provided by inspecting the plate under polarized light utilizing birefringence (Fig. 1b). This is used as a first guess for the distribution and magnitude of the initial molecular orientation where high or low values prevail in bright or dark regions, respectively. Mapping of this information to the FE model is accomplished by assuming a corresponding distribution of the maximum principal stretch λ_{max}^i (eigenvalue of $\boldsymbol{V}^i$, $\det\boldsymbol{V}^i = 1$). For simplicity five sections with different constant values of λ_{max}^i are considered. The direction of the orientation is assumed to be radial from the injection point

("gate"; see Fig. 1a). The plate is subjected to a temperature which is taken spatially uniform and increases with time. With increasing temperature the material flow resistance decreases and enables the "frozen-in" molecular stretch (and backstress) to relax. This spatially non-uniform re-deformation causes buckling of the plate. The deformed FE model is depicted in Fig. 3b and shows a qualitatively good agreement with the real plate in Fig. 1c.

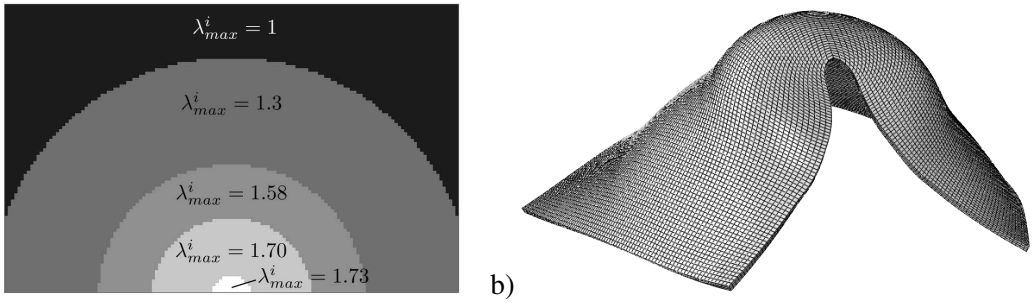

Figure 4: FE analysis of injection molded plate: a) distribution of initial molecular stretch, b) deformation after heating to 120° C

Conclusions

In this work a constitutive model for amorphous thermoplastic polymers is set up which incorporates an initial anisotropy and is able to describe the stress-strain response even above the glass transition. The model is used successfully to simulate a re-heating process of an injection molded plate. The resulting deformation of the plate is in good agreement with that observed in the real experiment. The correlation between the deformation of the real plate and the deformation obtained in the simulation evidences that the assumed initial molecular orientation and its mapping to the computational model is reasonable. However, while the flow field in the present case is quite obvious, it is hardly conceivable that this heuristic method is applicable to more complicated geometries. In that case one could use, for example, form filling simulations to map the initial state of the material to the FE model. Another subject of future work is the modification of the material model to capture the effect of strain rate dependent hardening at elevated temperatures caused by reptation of molecules in the entanglement network.

References

[1] Arruda, E. M.; Boyce, M. C.; Jayachandran, R., *Mechanics of Materials* **1995**, 19(2-3), 193-212

[2] Boyce, M.C.; Parks, D.M.; Argon, A.S., *International Journal of Plasticity* **1989**, 6, 593-615

[3] Boyce, M.C.; Weber, G.G.; Parks, D.M., *Journal of the Mechanics and Physics of Solids* **1989**, 37(5),647-665

[4] Limess, *Digital Image Correlation*. Q-400 Operation Manual, Krefeld 2009

[5] Struik, L.C.E., *Internal stresses, dimensional instabilities and molecular orientations in plastics*, John Wiley & Sons Ltd, Chichester 1990