

A FINITE STRAIN ELASTO-PLASTIC MATERIAL MODEL FOR SEMICRYSTALLINE POLYMERS INCORPORATING KINEMATIC AND ISOTROPIC HARDENING

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Abstract

Semicrystalline thermoplastic polymers e.g. Polyamide 6 (PA6), Polyetheretherketone (PEEK) have superior mechanical properties and are thus very important in numerous technically relevant applications. Reinforcing thermoplastic polymers with high performance continuous fibers e.g. carbon-, glass- or aramid fiber yields a composite material, which is producible into sheet formats that can be formed using thermoforming techniques. Parts made of thermoplastic fiber reinforced composites (TPFRCs) exhibit high strength to weight ratios and show the potential for shorter part cycle time and recyclability. During the thermoforming process of parts made of TPFRCs the “springback effect”, i.e. the undesired distortion of a part after unloading and removal from tooling, depicts a major problem. These shape distortions occur due to the formation of residual stresses on multiple scales. To accurately predict the residual stresses on the micro (matrix and fiber) scale, a constitutive model for the matrix material has to be developed.

Therefore, a phenomenological model formulation is proposed in this work, which is valid for large deformations and large deformation rates in the context of isothermal processes. To capture the biphasic nature of the polymer, i.e. to account for the amorphous and semicrystalline regions of the underlying microstructure, a parallel arrangement of both phases is applied. The overall material response is obtained by a rule of mixture. The qualitative validation of the hyperelastic, viscoplastic material model shows the promising potential to predict the formation and relaxation of residual stresses during the forming process of thermoplastic polymers.

1. Introduction

The binding forces between the molecule chains of thermoplastic polymers are the result of intermolecular van der Waals forces and mechanical entanglement. In contrast to thermoset polymers, which form irreversible chemical bonds throughout the curing process, thermoplastic polymers can therefore undergo repeated heating above the melting point and cooling cycles. Consequently, in numerous forming processes of parts made of thermoplastic polymers (e.g. extrusion or injection molding) the polymer is reshaped into the desired geometry after heating. Parts made of thermoplastic fiber reinforced composites (TPFRCs) are typically produced from blanks (so called organo sheets), where the fibers are already embedded in the matrix material. The part shape is obtained by heating the organo sheet above the melting temperature of the polymer and subsequently forming it under high pressure and in a short time. Despite the numerous benefits of TPFRCs (e.g. ease of storage of the

organo sheets, short part cycle times and recyclability), a major disadvantage is the process instability during forming. The formation of residual stresses on multiple scales due to temperature gradients and mismatches of coefficients of thermal expansion lead to undesired deformations of the part. This is referred to as the spring back effect.

Hence, in order to eliminate cost intensive and time consuming trial and error approaches, a strong demand for computational models arises, which accurately predict the material and structural response of the part during forming.

Therefore, a material model formulation for semicrystalline polymers, which is valid for large deformations in the context of isothermal processes, is presented in this work. To capture the evolution of residual stresses on the micro (fiber and matrix) scale, which are mainly driven by the different densities of amorphous and crystalline regimes, it is crucial to account for the biphasic nature of the polymer. In line with the work of Dusunceli and Colak [1], a parallel arrangement of amorphous and crystalline phase is chosen. Thus, the overall free Helmholtz energy is obtained by a rule of mixture of the energy contributions of both phases, where a constant degree of crystallinity serves as an input parameter. Thus, temperature or stress induced crystallization is not considered in the framework.

2. Material model formulation

To give a better understanding of the constitutive framework, Fig. 1 illustrates the modelling strategy in terms of a rheological model. As alluded above a parallel connection of both phases is considered.

To model the crystalline regime (highlighted in red in Fig. 1), a thermodynamically consistent, finite strain elasto-plastic material model, based on the formulation proposed by Vladimirov et al. [2, 3] in the context of metallic materials, is presented. Since the dependence of the spring back on the Bauschinger effect is well known, particularly for bend/unbend operations, isotropic and kinematic hardening are incorporated into the model. The kinematic hardening is of Armstrong-Frederick type and can be represented by means of a series connecting of an additional dashpot and the hardening spring in the rheological model. Introducing the pseudo viscosity $\eta^* = c/(\lambda b)$ which is depending on the hardening stiffness c , a dimensionless parameter b and the rate of plastic deformation $\dot{\lambda}$ yields nonlinear kinematic hardening in the case of plastic deformation ($\dot{\lambda} > 0$).

The amorphous phase (highlighted in blue, Fig. 1) is modeled by means of a thermodynamically consistent, visco-hyperelastic material formulation. The aforementioned is valid for large deformations and large deviations away from the thermodynamic equilibrium (i.e. large deformation rates) and in line with the work of Reese and Govingee [4]. Thus, within the rheological framework the amorphous phase can be represented by a Maxwell Element.

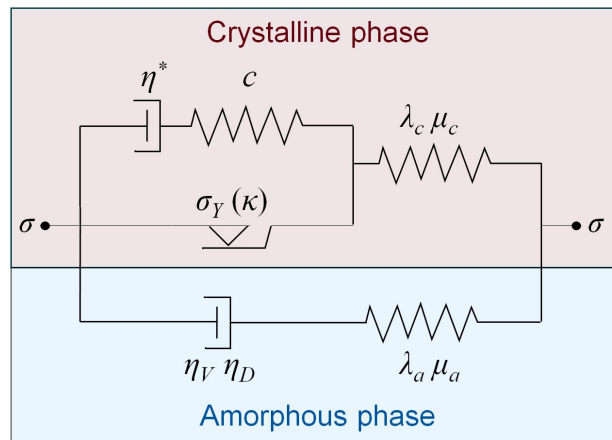


Figure 1. Modelling strategy: schematic illustration of the rheological model.

For the continuum-mechanical representation in the context of finite strains, several splits of the deformation gradient \mathbf{F} are introduced. The multiplicative decomposition of the deformation gradient $\mathbf{F}=\mathbf{F}_{ea}\mathbf{F}_i$ into an inelastic \mathbf{F}_i and elastic part \mathbf{F}_{ea} for the amorphous phase is in line with [4]. Following [2] and [5] the well-established split of the deformation gradient $\mathbf{F}=\mathbf{F}_{ec}\mathbf{F}_p$ into a plastic \mathbf{F}_p and elastic part \mathbf{F}_{ec} is performed for the crystalline phase. To account for the nonlinear kinematic hardening an additional multiplicative split of the plastic deformation gradient $\mathbf{F}_p=\mathbf{F}_{pe}\mathbf{F}_{pv}$ is carried out. Based on these operations, the following kinematic relations can be derived

$$\mathbf{C}_{ea} = \mathbf{F}_{ea}^T \mathbf{F}_{ea} = \mathbf{F}_i^{-T} \mathbf{C} \mathbf{F}_i^{-1}, \quad \mathbf{C}_{ec} = \mathbf{F}_{ec}^T \mathbf{F}_{ec} = \mathbf{F}_p^{-T} \mathbf{C} \mathbf{F}_p^{-1}, \quad \mathbf{C}_{pe} = \mathbf{F}_{pe}^T \mathbf{F}_{pe} = \mathbf{F}_{pv}^{-T} \mathbf{C}_p \mathbf{F}_{pv}^{-1} \quad (1)$$

Where \mathbf{C}_{ea} and \mathbf{C}_{ec} are the elastic right Cauchy-Green deformation tensors associated with the amorphous and crystalline phase, respectively. The right Cauchy-Green tensor is denoted by \mathbf{C} and the plastic right Cauchy-Green tensor by \mathbf{C}_p .

In order to derive the constitutive framework in a thermodynamically consistent manner the overall Helmholtz free energy is introduced and assumed to be obtained by the following rule of mixture.

$$\psi = \chi\psi_c + (1-\chi)\psi_a \quad (2)$$

Here, ψ_a and ψ_c are the energy contributions of the amorphous and crystalline phases. The degree of crystallinity is denoted by χ and assumed to be constant. An additive decomposition of the energy associated with the crystalline phase is postulated

$$\psi_c = \psi_{ec}(\mathbf{C}_{ec}) + \psi_{kin}(\mathbf{C}_{pe}) + \psi_{iso}(\kappa) \quad (3)$$

Where ψ_{ec} is the elastic energy density and ψ_{kin} and ψ_{iso} correspond to the stored energy due to kinematic and isotropic hardening, respectively. Here, κ denotes the isotropic hardening variable i.e. the accumulated plastic strain. The energy contribution stemming from the amorphous phase $\psi_a = \psi_{ea}(\mathbf{C}_{ea})$ is solely a function of the elastic energy contribution ψ_{ea} .

Following [2] and [4], the derivation of the second Piola-Kirchoff stress tensor \mathbf{S} as well as the set of evolution equations ($\dot{\mathbf{C}}_p$, $\dot{\mathbf{C}}_{pv}$, $\dot{\kappa}$, $\dot{\mathbf{C}}_i$) and thermodynamic conjugated driving forces is based upon the Clausius-Duhem form of the entropy inequality for isothermal processes.

Due to the deviatoric character of the flow rule, which is of von-Mises type, a volume preserving integration scheme for the internal variables associated with the plastic flow (\mathbf{C}_p , \mathbf{C}_{pv}) is required. To this end, an exponential map algorithm, based on the work of Dettmer and Reese [6], is applied for the numerical integration of the evolution equations. It is of note, that the presented model includes only symmetric tensor-valued internal variables. However, a local set of 5 nonlinear equations for the 5 unknowns (\mathbf{C}_p , \mathbf{C}_{pv} , $\Delta\lambda$, κ , \mathbf{C}_{pi}) has to be solved in an efficient manner by means of the Newton-Raphson method.

3. Numerical examples

In order to qualitatively validate the method and to provide an insight into the capabilities of the model, a simple virtual experiment is conducted. To this end, the proposed formulation is implemented as an user-defined material model (UMAT) into the finite element software ABAQUS.

Table 1. Material parameters.

| Crystalline phase | | | | | | Amorphous phase | | | |
|-------------------|-------------|-------|-----|------------|-------|-----------------|-------------|----------|----------|
| μ_c | λ_c | c | b | σ_0 | H | μ_a | λ_a | η_V | η_D |
| (MPa) | (MPa) | (MPa) | (-) | (MPa) | (MPa) | (MPa) | (MPa) | (MPa·s) | (MPa·s) |
| 1150 | 1730 | 50 | 2 | 500 | 50 | 192 | 288 | 100 | 100 |

The well-known Neo-Hookean form for the elastic energy contributions ψ_{ec} and ψ_{ea} is chosen, which depend on the Lamé constants λ_c, μ_c and λ_a, μ_a respectively. The volumetric and deviatoric viscosities, corresponding to the dashpot properties, are denoted by η_V and η_D . The set of material parameters is given in Table 1.

For the numerical investigation, a cubic specimen, which is fixed at both ends, is considered. A displacement is prescribed in longitudinal 1-direction and is increased linearly over the time. Subsequently, the displacement is held constant to allow for relaxation. The boundary conditions and loading procedure are depicted in the upper part of Fig. 2.

The results for this loading sequence are displayed in the lower part of Fig. 2. The reaction force time relation as well as the equivalent Cauchy stress for selected time steps is visualized, for a longitudinal cross section. With increasing displacement, stress concentrations in the center of the specimen can be observed, due to the lateral contraction. The latter ultimately lead to plastic deformation and corresponding necking. After one second the displacement is hold constant and stress relaxation, accompanied by additional necking, results in a further decrease of the reaction force.

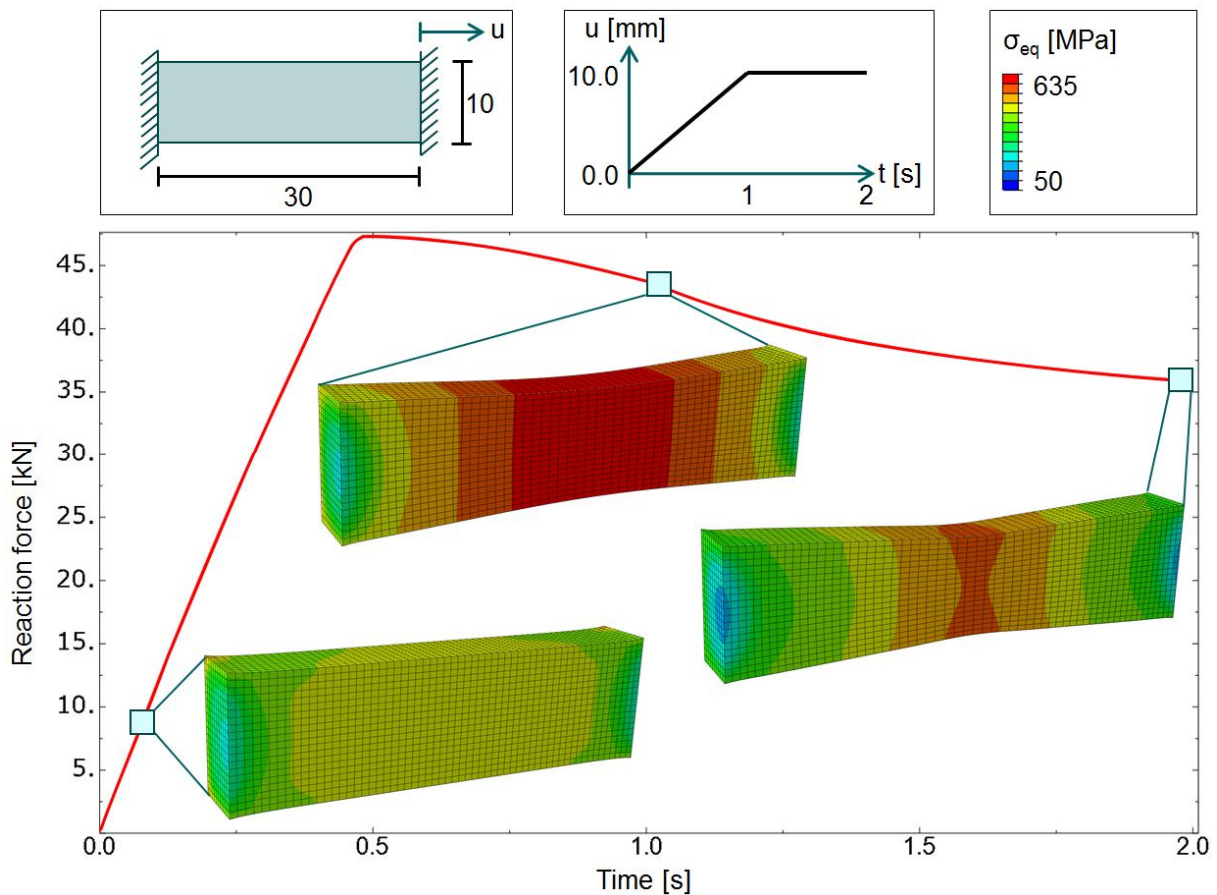


Figure 2. Reaction force time relation and equivalent Cauchy stress for selected time steps.

4. Conclusions

A flexible hyperelastic-viscoplastic material model for the prediction of semicrystalline polymers during mechanical loading is presented in this work. The model formulation is based on a phenomenological approach, where the biphasic nature of the polymer is captured by a rule of mixture. The framework is valid for large deformation as well as large deformation rates and accounts for

nonlinear kinematic hardening and isotropic hardening. To solve the set of nonlinear local equations an efficient and numerically robust solution scheme is applied.

The flexible framework allows the modelling of various different materials by specifying the form of the Helmholtz free energy contributions of the different phases and the hardening term. An expansion of the model to account for the parallel connection of several Maxwell elements within the amorphous phase is also straight forward from the theoretical point of view. However, this would lead to additional internal variables and hence additional evolution equations resulting in rising computational costs.

In order to quantitatively validate the method, the set of material parameters needs to be characterized based on experimental data for semicrystalline polymers. In the current framework the degree of crystallinity serves as a constant input parameter. To predict the formation of residual stresses during the thermoforming process, it is however crucial to account for the temperature induced crystallization. Thus, an appropriate crystallization kinetics model needs to be incorporated in the future. To account for the temperature dependence of the material and the evolution of the degree of crystallinity, thermomechanical coupling of the theory will be introduced in an upcoming work.

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