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Citation for published version (APA):
Janssen, R. P. M., Breemen, van, L. C. A., Pelletier, C. G. N., Govaert, L. E., & Meijer, H. E. H. (2006). Modelling large-strain deformation of thermo-rheologically complex materials : characterisation and validation of PMMA and iPP. In *13th International Conference on Deformation, Yield and Fracture of Polymers , April 10-13, 2006, Rolduc Abbey, Kerkrade, The Netherlands* (pp. 303-306)

Document status and date:
Published: 01/01/2006

Document Version:
Accepted manuscript including changes made at the peer-review stage

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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Modelling large-strain deformation of thermorheologically complex materials: Characterisation and validation of PMMA and iPP

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In this study an attempt is made to describe the thermorheologically complex deformation behaviour of the glassy polymer PMMA and semi-crystalline polymer iPP, by using a constitutive modelling approach [1]. For both polymers, it is shown that this approach successfully captures the thermorheologically complex behaviour of PMMA and iPP. Moreover, the model is capable of predicting yield stress and creep lifetime of PMMA using only one parameter set.

Introduction

Constitutive modelling is a useful tool to design and analyse polymer products without the need of costly experiments. Previous modelling work has already shown to be successful in describing the linear and visco-elastic deformation behaviour up to yield of polycarbonate (PC) [2]. A short-coming of this model was that only thermorheologically simple deformation behaviour, such as PC at room temperature and low strain rates, was captured. Deformation of thermorheologically simple materials is governed by only a single molecular relaxation process, i.e. the primary glass-transition (α-process). Many polymers, however, behave thermorheologically complex, which means that multiple relaxation processes contribute to the deformation, e.g. the secondary glass-transition (β-process) for polymethylmethacrylate (PMMA) or a contribution of the crystalline phase (ζ-process) for isotactic propylene (iPP). Also for PC at high deformation rates and low temperatures, the β-process contributes to the deformation. To describe the thermorheologically complex yield behaviour, Klompen and Govaert [3] extended the model of Tervoort et al. [2] by placing another Maxwell-element in parallel. In addition, attempts to describe the intrinsic post-yield behaviour of PC obtained by uni-axial compression testing by numerical modelling appeared to be successful too [4]. Later, Klompen et al. [5] showed that this description of the large strain deformation of PC led to accurate predictions of the yield stress, yield drop and draw ratio in the neck. Moreover, the same model is able to predict the creep life-time of PC samples with different thermo-mechanical histories [6]. The strength of this approach is that the age of the materials is accounted for by only one material parameter S_a, which is easily determined by tensile testing. Recently, this model is extended to describe thermorheologically complex behaviour by modifying the viscosity function [1]. In this study, a characterisation of PMMA and iPP is performed by compression testing and micro indentation to obtain the model parameters, as well as the performance of the thermorheologically complex implementation is validated by predictions on results of tensile testing and creep testing.

Materials and Methods

The materials investigated are PMMA (Röhm GmbH, Plexiglas, type unknown) supplied as 6 mm diameter extruded rod, and iPP (Borealis A/S, HD120M0) supplied as granules. The iPP granulate were compression moulded at 240°C into 200x200x5 mm^3 plates. For the uni-axial compression tests, cylindrical samples of ∅6x6 mm (PMMA) and ∅4x4 mm (iPP) were machined from the extruded rod and compression moulded plates, respectively. Two grades of PMMA were injection moulded into tensile bars according to ASTM-D638, having a different thermal history. To obtain tensile bars of iPP, the plates were levelled off equally on both sides to a 1.5mm thick plate. Subsequently, dog-bone shaped samples were cut from these plates. Uni-axial compression tests, tensile tests and creep tests were performed on a servo-hydraulic MTS Elastomer Testing System 831. During these experiments the temperature was kept constant at 20°C in a temperature chamber.

Results

Characterisation of PMMA

The model parameters are determined from the material's intrinsic deformation. A way to obtain this true stress-strain behaviour is by compression testing, where localisation phenomena, such as crazing and necking, are absent. The results of compression tests on PMMA performed at rates of $3\cdot10^{-5} - 10^{-1}$ s^{-1} are shown in figure 1a. This figure clearly shows the thermorheologically complex nature of PMMA. At low strain rates ($3\cdot10^{-5} - 10^{-3}$ s^{-1}), only one molecular process accounts for the deformation behaviour (dotted lines), but at the high strain rates the increase in yield stress with strain rate is larger due to the additional contribution of the β-process (solid lines). Another crucial observation is the dramatic softening at the highest strain rates ($10^{-2} - 3\cdot10^{-1}$ s^{-1}) initiated by deformation induced heating. The α-parameters are obtained from fitting on the lowest 4 strain rates, whereas the β-parameters are collected from fitting on the other strain rates. Results can be seen in figure 1b. The model accurately captures post-yield deformation in both the α- and α-and-β-regime. Furthermore, the values of the experimental yield stresses are compared to the yield stress predictions in figure 2a. Also this figure confirms that the current modelling approach accurately describes thermorheologically complex behaviour of PMMA. The pressure dependence parameter μ of PMMA is determined by micro indentation. Figure 2b compares the experimental data to indentation results obtained by the model for different values of μ. It can be seen that a value of 0.13 gives the best result. The complete set of material parameters is given in table 1.1.

Table 1.1: Material parameter set of PMMA

E [MPa]	ν [-]	$\eta_{0,\alpha}$ [MPa·s]	$\eta_{0,\alpha+\beta}$ [MPa·s]	$\tau_{0,\alpha}$ [MPa]	$\tau_{0,\alpha+\beta}$ [MPa]	μ [-]	S_a [-]	G_r [MPa]
900	0.4	$5.22\cdot10^{6}$	$6.91\cdot10^{5}$	2.9	6.4	0.13	-	26

Validation: Predictions on PMMA

To validate the model's capabilities, tensile tests are performed on tensile bars of two grades of PMMA with a different thermal history. First, the age S_a of the two grades is determined by a tensile test at a reference strain rate of 10^{-4} s^{-1}, which is the reference point in figure 3a. The initial S_a values are 6.2 and 7.4, respectively. Using these values, it can be seen in figure 3a that for both grades of PMMA the predicted yield stresses compare well to the experimental obtained values. In addition, an attempt was made to predict the creep lifetime of PMMA. The results in figure 3b show that also the creep lifetime of both grades of PMMA is predicted accurately by the model.

Characterisation and validation of iPP

Within the range of applied strain rates, the deformation of iPP at room temperature is controlled by both the α-process and the ζ-process. At elevated temperatures, however, the material behaves thermorheologically simple at the lower strain rates. This can be seen in figure 4a, which shows the yield stress data vs. strain rate of compression testing at 20°C and 60°C. Therefore, the α-parameters are derived from the compression testing at 60°C, whereas the results obtained 20°C yielded the β-parameters. For iPP, the micro indentation experiments on iPP did not show reproducible results, most probably due to its semi-crystalline composition. Consequently, the pressure dependence parameter μ is determined from yield stress data under hydrostatic pressure taken from literature [7, 8], as shown in figure 4b. This gives a value of 0.15 for the pressure dependence μ of iPP. Figure 5a shows that the model captures the thermorheologically complex true stress-strain behaviour of iPP. Using this parameter set, also the tensile yield stress is accurately predicted as shown in figure 5b. The model parameters of iPP are given in table 1.2.

Table 1.2: Material parameter set of iPP

E [MPa]	ν [-]	$\eta_{0,\alpha}$ [MPa·s]	$\eta_{0,\alpha+\zeta}$ [MPa·s]	$\tau_{0,\alpha}$ [MPa]	$\tau_{0,\alpha+\zeta}$ [MPa]	μ [-]	S_a [-]	G_r [MPa]
900	0.4	$2.32\cdot10^9$	$1.16\cdot10^8$	1.16	1.87	0.15	5	1.7

Conclusions

The new viscosity function successfully describes the thermorheologically complex deformation behaviour of PMMA and iPP. Moreover, the model predicts the tensile yield and creep life-time of multiple grades of PMMA using the same parameter set.

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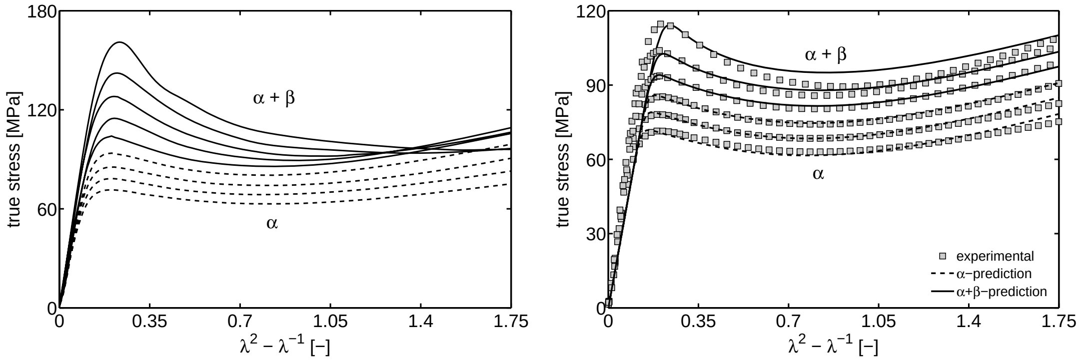
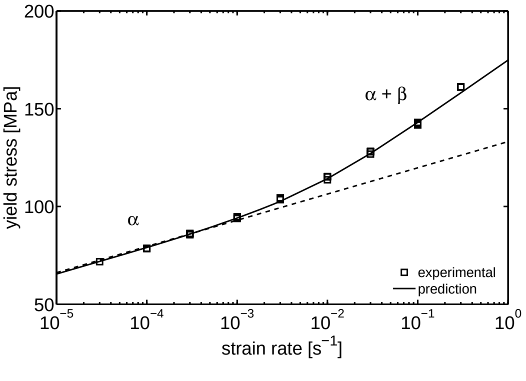


Figure 1: a) Intrinsic deformation behaviour of PMMA in both α–regime and α+β–regime b) Model predictions (lines) compared to experimental curves (squares).



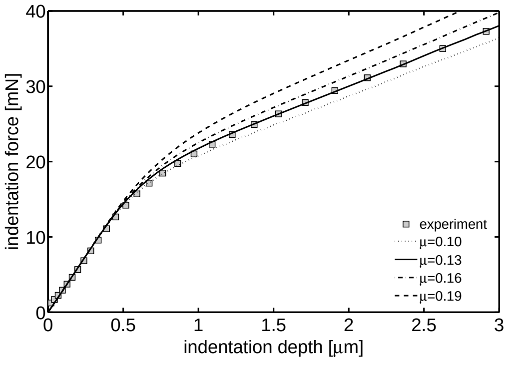


Figure 2: a) Yield stress predictions (line) compared to experimental data (squares) of PMMA b) Pressure dependence parameter μ of PMMA determined from micro indentation.

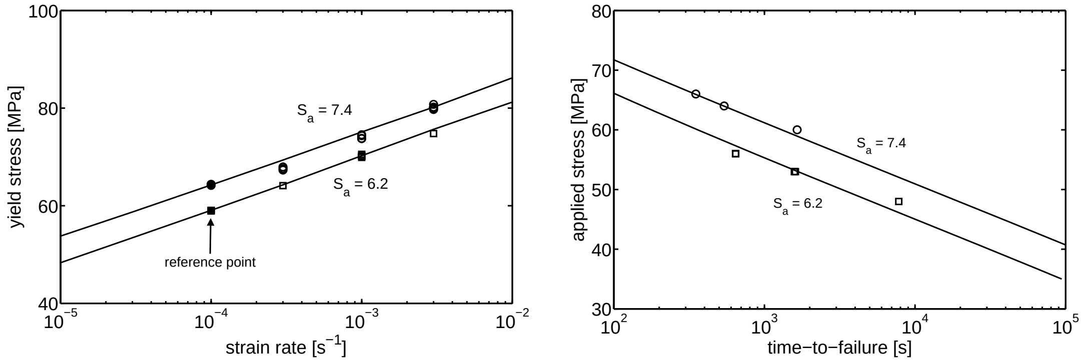


Figure 3: a) Tensile yield stress predictions and b) Creep life-time prediction of two grades of PMMA correspond well with experimental results.

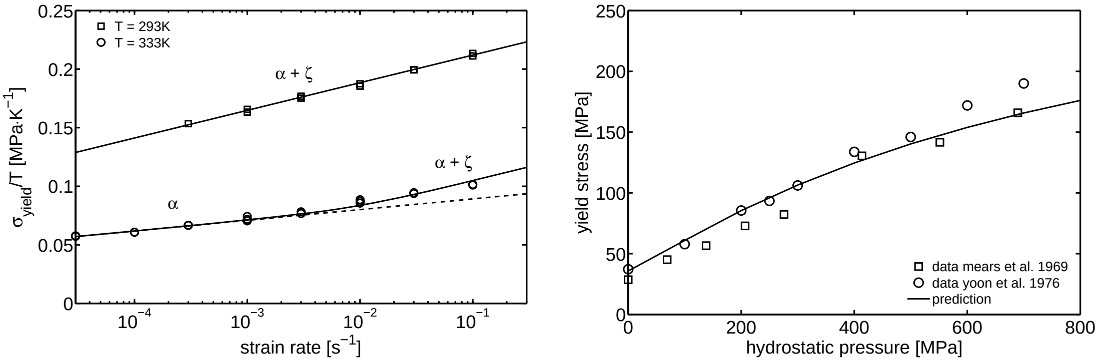


Figure 4: a) a) Yield stress predictions (line) compared to experimental data (squares) of iPP b) Tensile yield stress predictions of iPP.

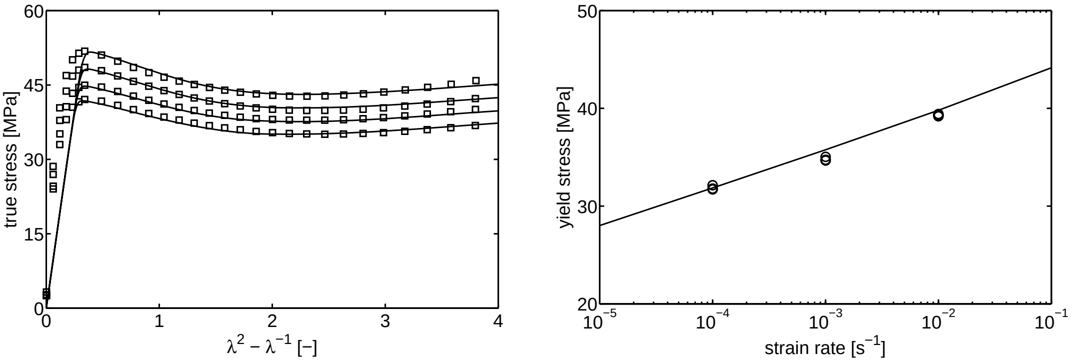


Figure 5: a) Description of the intrinsic deformation behaviour of PP in α+ζ–regime, b) Tensile yield stress predictions.