Prediction of yield stress development using structural relaxation

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Introduction

In previous work [1] we showed that by extrapolating the results of the development of yield stress due to annealing treatments on a glassy polymer below the glass transition temperature, T_g, towards the development of properties during processing, we were able to predict the resulting distribution of yield stresses. In this previous approach, however, T_g was used as an input parameter. In the approach presented here [2], structural relaxation kinetics are used to describe the relaxation kinetics of the solidifying glass, and thus describing T_g.

TNM-Model

Structural relaxation has already been extensively used to describe a number of relaxation phenomena observed in polymers, e.g. volume and enthalpy. In figure 1 (left) relaxation of a property P (volume) with temperature is shown. Figure 1 (right) shows how this can be translated to the relaxation of the zero-viscosity.

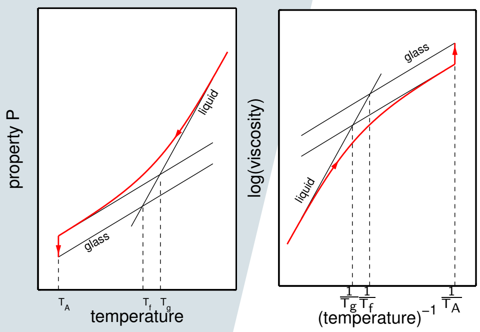

Figure 1 *Relaxation kinetics: annealing temperature, T_a, fictive temperature, T_f and glass transition temperature, T_g*

In our approach we apply the Tool-Narayanswamy-Moynihan (TNM) model to the retardation of the zero-viscosity. The zero-viscosity is used rather than the yield stress itself, since the zero-viscosity is loading rate and -geometry independent. The equations describing the yield stress by means of the TNM model can be summarized as follows:

$$T_f(T,\xi) = T - \int_0^{\xi} M_P(\xi-\xi')\frac{dT}{d\xi'}d\xi' \quad (1)$$

$$M_P(\xi) = \exp\left(-\left(\frac{\xi}{\tau_{Pr}}\right)^{\beta}\right) \qquad \xi(t) = \tau_{Pr}\int_0^t \frac{dt'}{\tau_P(T,T_f)} \quad (2)$$

$$\tau_P(T,T_f) = A\exp\left(\frac{x\Delta H}{RT} + \frac{(1-x)\Delta H}{RT_f}\right) \quad (3)$$

$$\log_{10}(\eta_0(T,\xi)) = \log_{10}\left(\frac{A_0(S_a)R}{V^*}\right) + \log_{10}(T) + \frac{1}{2.303}\left(\frac{\Delta U_l}{R}\right)\frac{1}{T} + \frac{1}{2.303}\left(\frac{\Delta U_l - \Delta U_g}{R}\right)\left(\frac{1}{T_f(\xi)} - \frac{1}{T}\right) \quad (4)$$

$$\sigma_y = \sigma_s + \sigma_r \quad (5)$$

$$\sigma_s = 3\eta\dot{\epsilon}_0 \quad ; \quad \sigma_r = G_r(\lambda_y^2 - \lambda_y^{-1}) \quad (6)$$

Experimental

From a commercial grade of polycarbonate, Lexan 141R, injection molded samples were made. Mold temperatures were varied from 30°C to 130°C. Subsequently tensile bars were machined from the injection molded samples to determine the resulting yield stress, see figure 2 below.

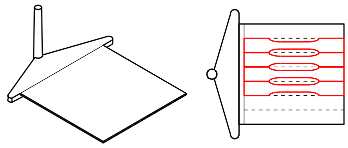

Figure 2 *Injection molded part and tensile bars made thereof*

Results

The results show that both annealing close to T_g, and prediction of the yield stress distribution as it develops due to processing conditions can be described accurately by our approach.

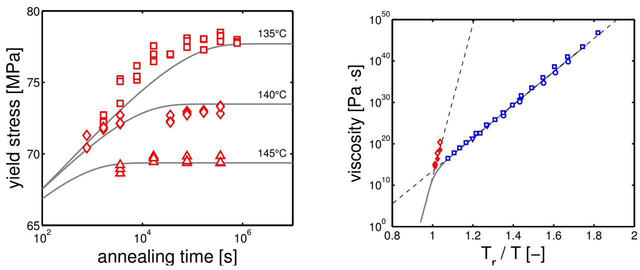

Figure 3 *Annealing close to T_g: symbols are experimental results, lines are model predictions (left); development of zero viscosity versus temperature, T_r is a reference temperature, here equal to T_g (right)*

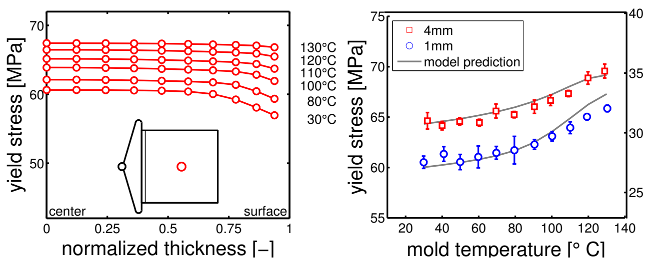

Figure 4 *Distribution of the yield stress over the normalized part thickness (left); experimental yield stresses versus model predictions (right)*

Conclusions

With the use of structural relaxation kinetics yield stresses can be predicted from processing conditions. This makes it possible to design a product for performance without ever doing a single experiment.

References:

[1] Govaert, L.E., Engels, T.A.P., Klompen, E.T.J., Peters, G.W.M., Meijer, H.E.H.: Processing induced properties of glassy polymers: Devolopment of the yield stress in polycarbonate. (IPP, XX(2), 170-177, (2005))

[2] Engels, T.A.P., Govaert, L.E., Peters, G.W.M., Meijer, H.E.H.: Processing induced properties in glassy polymers: application of structural relaxation to yield stress development (J.Polym.Sci., part B, Polym.Phys., submitted (2005))

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