A constitutive model for semi-crystalline polymers: A multiple viscoelastic relaxation processes implementation.

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ABSTRACT

The constitutive modelling of semi-crystalline polymers seeks to obtain reliable predictive tools for a wide range of their mechanical responses. Such efforts have continued to occupy computational material scientists. Although significant advances have been made regarding amorphous polymers, thanks to works by Buckley [1], Boyce [2], and Govaert [3], there is significant research scope for developing similar predictive modelling fidelity for semi-crystalline polymers. The presence of crystalline and amorphous phases in semi-crystalline polymers presents interesting constitutive modelling challenges.

In this study, a physically based, three-dimensional constitutive model has been developed for simulating a wide range of features observed in deformation and processing of semi-crystalline polymers. The constitutive mathematics is based on a one-process *Grass-Rubber* model for amorphous polymers proposed by Buckley and colleagues [1]. The model philosophy exploits the presence of multiple relaxation processes associated with the different mechanics of the crystalline, amorphous and pseudo-amorphous parts of the polymer. The model development reasoning is inspired by a well-known physical framework of rate-dependent deformation that establishes a correlation between the observed transition in flow stress of a material and the secondary β-transition of the viscoelastic behaviour. Here, two dominant relaxation processes were identified - the α- and the β-processes. Each process was modelled using the bond-stretching and conformational stresses constitutive mathematics of the *Glass-Rubber* model.

The model has been implemented numerically into a commercial finite element code through a user-defined material subroutine (UMAT) and validated against compression test results carried out on an isotactic polypropylene across an unusually wide range of strain rates [4]. In this study, the model predicts quite well the experimentally observed nonlinear mechanical responses like: temperature- and rate-dependence, adiabatic heating effects, structural rejuvenation and post-yield de-ageing of polypropylene. It provides a viable modelling tool that can be utilized for design involving semi-crystalline polymers at room temperature as well as exploring the processing response at elevated temperatures.

REFERENCES

[1] Buckley C. Glass-rubber constitutive model for amorphous polymers near the glass transition. *Polymer* (Guildf) 1995;36:3301–12. doi:10.1016/0032-3861(95)99429-X.

[2] Mulliken AD, Boyce MC. Mechanics of the rate-dependent elastic–plastic deformation of glassy polymers from low to high strain rates. *Int J Solids Struct* 2006;43:1331–56.

[3] Tervoort TA, Klompen ETJ, Govaert LE. A multi-mode approach to finite, three-dimensional, nonlinear viscoelastic behavior of polymer glasses. *J Rheol* (N Y N Y) 1996;40:779–97.

[4] Okereke MI, Buckley CP, Siviour CR. Compression of polypropylene across a wide range of strain rates. *Mech Time-Dependent Mater* DOI 101007/s11043-012-9167-Z 2012:1–19. doi:10.1007/s11043-012-9167-z.