

Visco-plastic behaviour of a polymer matrix at the fibre diameter length scale: a finite element mesoscale model relying on shear transformation zone (STZ) dynamics

Nathan Klavzer^{1*}, Frederik Van Loock¹, Jérémy Chevalier², Laurence Brassart³, Thomas Pardoën¹

¹Institute of Mechanics, Materials and Civil Engineering (iMMC), UCLouvain, Place Sainte Barbe 2, Louvain-la-Neuve 1348, Belgium

²Solvay, Rue de Ransbeek 310, Neder-Over-Heembeek 1120, Belgium

³ Department of Engineering Science, University of Oxford, Parks Road, Oxford OX1 3PJ, United Kingdom

* nathan.klavzer@uclouvain.be

Polymeric glasses exhibit complex behaviour when subjected to deformation below the glass transition temperature. Uniaxial stress-strain curves typically include post-yield strain softening, strain hardening, and non-linear unloading. In addition, the deformation and failure responses are sensitive to the rate of deformation, pressure, and temperature. Sophisticated (visco-)elastic-(visco-)plastic continuum constitutive models have been developed to simulate the large strain deformation of (glassy) polymers; they generally give excellent fits to uniaxial stress-strain curves. However, they require the calibration of a large number of mostly phenomenological parameters, give limited insights into failure, and struggle to accurately predict the response for more complicated loading states and histories. At the opposite scale, molecular dynamics (MD) simulations have been used to elucidate the discrete molecular deformation mechanisms leading to the heterogeneous inelastic behaviour of polymeric glasses. The results of MD calculations suggest that plastic deformation of polymeric glasses is caused by thermally activated molecular rearrangements and conformational changes of a collection of polymer chains parts.

The use of a mesoscale numerical model based on the activation of shear transformation zones (STZs) offers a convenient approach to bridge continuum and molecular dynamics simulations, which are typically limited to small length and time scales. We have used the implementation by Homer and Schuh [1] of Argon's STZ theory [2] to develop a mesoscale finite element model for polymeric glasses. It is assumed that the elementary deformation mechanism giving rise to macroscopic plastic deformation in a polymeric glass is a pure shear deformation of an STZ; this corresponds to a change in molecular conformational state. Plastic deformation is governed by these changes and their interaction with the surrounding (visco-)elastic matrix. The mesoscale STZ framework requires the calibration of only five parameters and successfully predicts the complex large deformation response of glassy polymers, including creep and non-linear unloading [3]. In this contribution, we will summarise the key building blocks of the mesoscale framework and discuss a possible route for model calibration. In addition, we discuss the role of the visco-elastic matrix on the model predictions. These insights can be used to simulate the time- and temperature-dependent visco-plastic deformation and failure response of a fibre-reinforced polymer composite matrix at the fibre-diameter length scale.

References

[1] E.R. Homer and C. A. Schuh, *Acta Materialia*, 57(9), 2823-2833, 2009.

[2] A. S. Argon, *Acta Metallurgica*, 27(1), 47-58, 1979.

[3] J. Chevalier, L. Brassart, F. Lani, C. Bailly, T. Pardoën, and X. P. Morelle, *Journal of the Mechanics and Physics of Solids*, 121, 432-446, 2018