MICROMECHANICAL MODELLING OF THE DEFORMATION KINETICS OF SEMICRYSTALLINE POLYMERS

J.A.W. van Dommelen[a)], A. Sedighiamiri, L.E. Govaert
Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

Summary An elasto-viscoplastic two-phase composite inclusion-based model for the mechanical performance of semicrystalline materials has previously been developed. This research focuses on adding quantitative abilities to the model, in particular for the stress-dependence of the rate of plastic deformation, referred to as the yield kinetics. A key issue in achieving that goal is the description of the rate-dependence of slip along crystallographic planes.

INTRODUCTION

The elasto-viscoplastic behaviour of semicrystalline polymeric materials is strongly dependent on the underlying microstructure consisting of both amorphous and crystalline domains [1, 2]. A micromechanically-based model for the constitutive behaviour of semicrystalline polymeric material has been presented in Van Dommelen et al. [3]. The model accounts for both crystallographic and morphological texture, the latter corresponding to the orientation distribution of the lamellar interface normals. A three-level modelling approach was used to study intraspherulitic deformation and stresses for semicrystalline polyethylene [4] and to predict the response of tensile specimens obtained at different angles with respect to the extrusion direction of the material [5]. The current research focuses on adding quantitative abilities to the micromechanical model, in particular for the stress-dependence of the rate of plastic deformation, referred to as the yield kinetics.

MODEL DESCRIPTION

The constitutive behaviour of semicrystalline material is modelled by an aggregate of two-phase composite inclusions. This composite inclusion model is discussed in detail in [3]. Each inclusion consists of a crystalline and an amorphous phase. A microstructural elasto-viscoplastic constitutive model is defined for both the crystalline and the amorphous phase, where the plastic deformation of the crystalline phase is described by a rate-dependent crystal plasticity model. To relate the volume-averaged mechanical behaviour of each composite inclusion to the imposed boundary conditions for an aggregate of inclusions, a hybrid local-global interaction law is used [3].

TOWARDS A QUANTITATIVE STRUCTURE-PROPERTY RELATIONSHIP

In order to predict both the short- and long-term failure of polymers, quantitative predictions of the yield kinetics of these materials are required. The present work is directed towards the prediction of the yield and post-yield behaviour, and texture evolution in semicrystalline polymers during large deformations at different strain rates. A critical factor is the stress-dependence of the rate of plastic deformation, the slip kinetics, which is the mechanism underlying time-dependent, macroscopic failure. The kinetics of the macroscopic plastic flow strongly depend on the slip kinetics of the individual crystallographic slip systems. Therefore, an accurate quantitative prediction requires a proper description of the rate-dependence of slip along crystallographic planes. As a first step in achieving this goal, the previously used viscoplastic power law relation is replaced with an Eyring flow rule. The re-evaluation of the slip kinetics is performed using a combined numerical/experimental approach and the refined slip kinetics are then validated for uniaxial compression data of isotropic HDPE, for different strain rates [6].

A double yield phenomenon is found in the model prediction and is related to morphological changes that induce a change of deformation mechanism, see Figure 1. For polyethylene, a double yield point is also experimentally observed during both tensile and compressive deformation modes. In literature, several possible mechanisms have been proposed to explain this behaviour, among which different deformation processes for the first and second yield point, often associated with fine slip and coarse slip. Even though the present model considers only fine slip, it mimics this complex behaviour, where it is observed that after the first yield point a change in the mechanisms occurs and transverse slip systems become active, whereas the primary chain slip mechanism was the dominant process around the first yield point.

The description of the slip kinetics is further refined in order to predict the temperature dependence of the kinetics of yield for polyethylene. The experimental data in Figure 2 show the presence of two different processes, where one can be attributed to the crystalline phase and the other to the alpha-relaxation mechanism in the amorphous phase. Also shown in this figure is a prediction of the temperature dependence of the macroscopic yield kinetics as well as time-to-failure in creep experiments with the micromechanical model.

[a)] Corresponding author. E-mail: J.A.W.v.Dommelen@tue.nl.

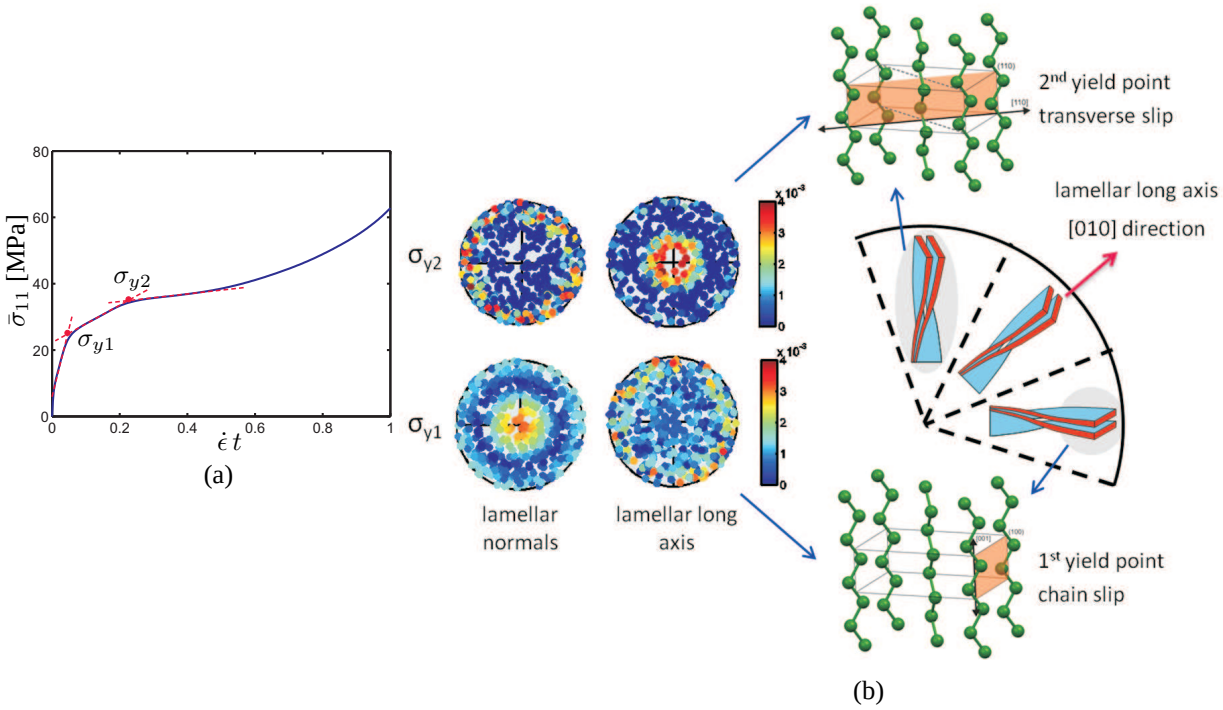

Figure 1. (a) Double yield behaviour predicted by the micromechanical model and (b) microstructural origin of double yield prediction.

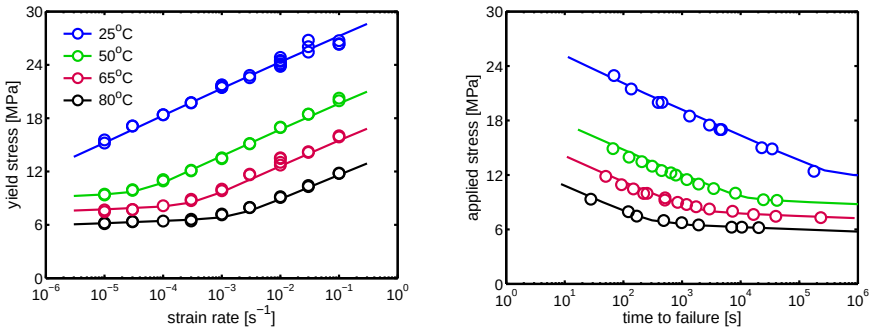

Figure 2. Temperature dependence of (a) yield kinetics and (b) time-to-failure of HDPE (markers) and predicted by the micromechanical model (solid lines).

CONCLUSIONS

The current research focuses on adding quantitative abilities to a micromechanical constitutive model for semicrystalline polymers, in particular for the stress-dependence of the rate of plastic deformation, referred to as the yield kinetics. A key issue in achieving that goal is the description of the rate-dependence of slip along crystallographic planes. The slip kinetics have been re-evaluated and characterized using a hybrid numerical/experimental procedure, and the results were validated for uniaxial compression data of isotropic HDPE, at various strain rates. A double yield phenomenon is observed in the model prediction and texture analysis shows that the double yield point in the model can be related to morphological changes during deformation, that induce a change of deformation mechanism. In addition, the temperature dependence of the kinetics of yielding has been described.

References

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