Micromechanically based modeling of the yield kinetics of semicrystalline polymers

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Introduction
The mechanical behavior of semicrystalline polymers is strongly dependent on their crystallinity level, the initial microstructure (see figure 1) as well as the evolution of this microstructure during deformation.

![Figure 1. Variation in microstructure over the thickness of injection molded HDPE, and the resulting different mechanical response [1].](image)

The principal objective of this study is quantitative prediction of deformation kinetics of semicrystalline polymers, using a multi-scale, micromechanical model [2].

Micromechanical model
At the microscopic level, the heterogeneous material is idealized by a two-phase composite entity [1], comprised of a crystalline lamella, which plastically deforms by rate-dependent crystallographic slip, and an amorphous layer, with plastic flow being a rate-dependent process. The material at the macroscopic level is modeled by an aggregate of a discrete number of these composite inclusions. A hybrid local-global interaction law is used to relate the mechanical response of each entity to that of the aggregate. The model is schematically show in figure 2.

![Figure 2. Schematic representation of the micromechanical model.](image)

Results and discussion
A critical factor in adding quantitative predictive abilities to the model, is a proper description of the stress-dependence of the rate of plastic deformation, referred to as slip kinetics. To do that, the previously used power law relation is replaced with an Eyring flow rule. The slip kinetics, are then re-evaluated using a hybrid numerical/experimental approach. A double yield phenomenon is observed in the model prediction (figure 3), and is related to the morphological changes, that induce a change of deformation mechanism, from the chain slip at the first yield point to the transverse slip at the second yield point.

![Figure 3. Predicted tensile stress-strain curve (left), and activity of the chain slip at the first yield point (middle top) and the transverse slip at the second yield point (middle bottom). The color represents the magnitude of the resolved shear rate of each inclusion. Schematic representation of the active slip systems within a spherulite at each yield point (right).](image)

Predicted compressive true stress-strain curves at varying strain rates, using the refined parallel slip kinetics, and the crystallinity dependence of the compressive first and second yield stress, are shown in figure 4.

![Figure 4. The predicted true stress-strain curves compared to experimental data (left), and crystallinity dependence of the two yield points predicted by model, compared to experimental data (right).](image)

Conclusion
Deformation kinetics of semicrystalline polymers were quantitatively predicted as a function of crystallinity and microstructure, using a micromechanical approach. A double yield phenomenon was predicted using only fine slip and the compressive response were predicted well, up to lamellar fragmentation.

References