Micro-mechanical modelling of oriented Polyethylene

S.M. Mirkhalaf, J.A.W. van Dommelen, L.E. Govaert, M.G.D. Geers

Introduction
During some manufacturing processes for polymeric products, such as injection molding or film blowing, the material is under shear and elongational flow resulting in an oriented microstructure after crystallization which leads to anisotropic mechanical behaviour. The objective of this work is to model the orientation induced anisotropic behaviour of semi-crystalline HDPE.

Micro-mechanical model
At the microscopic level, the material is considered to be composed of amorphous and crystalline phases forming a composite inclusion as shown in Figure 1.

![Figure 1: A composite inclusion composed of a crystalline lamella and an amorphous phase.](image1)

The deformation behaviour of the material is obtained as the volume average of the response of an aggregate of composite inclusions, using a hybrid mean-field approach. In hot-drawn tapes, the crystalline domains show a preferred orientation distribution. Figure 2 shows the orientation distribution of a sample of drawn HDPE with a draw ratio of 4.

![Figure 2: Pole figures of the orientation distribution of HDPE samples with draw ratio of 4.](image2)

As can be seen in Figure 4, in spite of considering the oriented crystallographic structure, the tensile yield kinetics are not well captured specially when the sample is cut in the machine direction. This signifies that in addition to the crystallographic orientation, an oriented amorphous phase should also be introduced. As suggested and used by Poluektov et al. [2] the pre-stretched included EGP model has been adopted for the oriented amorphous phase of oriented HDPE tape. A pre-stretching of the amorphous network in this model leads to an internal pre-stretched state.

Preliminary results
Simulations are performed on oriented HDPE tape at room temperature under strain rate of $\dot{\varepsilon} = 0.0001$ (1/s) and at different loading angles. Figure 5 depicts a comparison of the yield stresses obtained in the experimental results and simulations. Simulations are conducted with and without considering amorphous anisotropy.

Figure 4: Tensile yield kinetics of HDPE samples with draw ratio equal to 4 considering only the crystallographic orientation (assuming an isotropic amorphous phase), symbols: experiments and lines: simulations [1].

![Figure 5: Tensile yield kinetics of HDPE samples with draw ratio equal to 4 (symbols: experiments, lines: simulations).](image5)

Conclusion and future research
The modified micro-mechanical model, including a pre-stretched EGP model, will be used to capture the effect of a pre-oriented amorphous phase on the overall response of oriented HDPE films with different draw ratios, under different strain rates and eventually different temperatures. The model predictions will be compared more comprehensively against experimental results.

References: