Micromechanical modeling of elastic properties in polyolefins

Proposed topic: Structure development during processing

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During the part forming, the stretching or the shearing of the polymer melt under strong cooling conditions lead to a flow-induced crystallization, which generates specific crystalline morphologies such as deformed spherulites, shish–kebab or more complex crystalline macrostructure like in polypropylene. The induced crystalline orientation and the amount crystallinity are with high influence with the anisotropy and the strong variation of the mechanical properties. Now, process simulations including a flow-induced crystallization law coupled to a viscoelastic behavior based on molecular models allow predicting the final crystallinity and the final molecular orientation in the crystalline phase. But, from the predicted crystalline morphology of the polymer, little was done to predict the mechanical properties.

The aim of this work is determine the mechanical properties of isotropic semi-crystalline polymers from the knowledge of the mechanical properties of its two phases by micromechanics modeling. Semi-crystalline polymers are heterogeneous materials, which are be assumed in this work as crystallites embedded into an amorphous phase. Considering an isotropic isotactic polypropylene PP and an isotropic high density polyethylene HDPE, the HDPE shows a lower modulus than the PP despite a higher crystallinity and higher elastic properties for both phases. This paradox can be explained by micromechanics modeling by taking into account the crystallite geometry. Two models are especially chosen for their theoretical ability to represent semi-crystalline polymers: a differential scheme matrix/inclusion model and a self-consistent scheme composite inclusion aggregate. In the first model, the material is represented by randomly distributed ellipsoidal crystallites embedded in an amorphous matrix, while in the second one, it is an aggregate of randomly oriented two-layered-phase composite inclusions (crystalline/amorphous). Computed results compared to experimental data prove the effectiveness of matrix/inclusion model in representing the elastic properties for both polymers. Moreover, the model will demonstrate the high influence of the crystalline lamella aspect ratio on the elastic properties of semi-crystalline polymers.