Multiscale Modeling of Polymer Crystallization

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Abstract

Introduction: The manufacturing of high quality injection molded parts requires a deep understanding of material properties, process parameters and product design. The behavior of a polymer during the injection molding process and the performance of the final part are strongly determined by the material structure formed during filling and cooling. During processing, a polymer is normally subject to a complex thermo-mechanical history that leads to different microstructures at different locations, because of variations in shear rate, pressure and temperature. The prediction of the final microstructure is very important to attain manufacturing processes in which defects such as uncontrolled warpage, incorrect part dimensions, excessive weight, etc. are absent. Predicting the microstructure requires the simulation of the crystallization process which is a complex problem because it is necessary to combine transport phenomena of the multi-phase flow in non-isothermal conditions with crystallization kinetics. This requires the calculation of polymer properties on a microscopic scale using information from a macroscopic scale. It is possible to define this problem as a multi-scale materials design problem.

Framework: The main objective of the presented work is to describe the crystallization kinetics of semi-crystalline thermoplastics with a multiscale model implemented into COMSOL Multiphysics® software. This is done by identifying the analytical parameters needed to connect crystallization kinetics with molecular material properties and applying the analytical scheme to the numerical simulation during filling and cooling in an injection molding process. The filling and cooling simulations, implemented by using the CFD and Heat Transfer Modules, requires the simultaneous solution of non-Newtonian multi-phase flow (polymer/air) and thermal fields in non-isothermal condition and transient regime. The COMSOL Multiphysics® simulations are linked to the in-house developed code SphäroSim. This code used the results of the macroscale injection molding simulation as input data and it is based on cellular automata for calculation of crystallization kinetics. The numerical method, crystallization kinetics and their implementation into numerical software are described as well as the experimental data (Figure 1).

Results: The validation of the numerical model was performed by comparing simulation predictions with experimental tests. The results of isotactic polypropylene show a good agreement in predicting the fountain flow effect and the difference in temperature profiles. during filling. The different material morphologies after cooling are reported in Figure 2, pointing-out the flow- and thermal induced microstructures. The link between COMSOL Multiphysics® and SphäroSim is possible by converting the results of the filling and cooling simulation to the

OpenSource file format VTK (Visualization Toolkit) and use them as boundary conditions in the microstructure simulation. This allows the time resolved calculation of the crystallization process and a prediction of the final microstructure in the part (Figure 3) which can be used in further simulations such as a structural analysis.

Conclusion: The crystallization kinetics was successfully simulated. Application to isotactic polypropylene illustrates the complexity of modeling the different material microstructures using COMSOL-SphäroSim integration.

Reference

Kim K.H., Isayev A.I., Kwon K., Flow-induced crystallization in the injection molding of polymers: A thermodynamic approach. J. of Applied Polymer Science, 2005, 95:502-523.
Rong. Y., He H.P., Cao W., Shen C.Y., Chen J.B., Multi-scale molding and numerical simulation of the flow-induced crystallization of polymer. Computational Material Science, 2013, 67:35-39.
Zheng. R., Tanner R.I. et al., Modeling of flow-induced crystallization of colored polypropylene in injection molding. Korea-Australia Rheology Journal, 2010, 22:151-162.

Figures used in the abstract

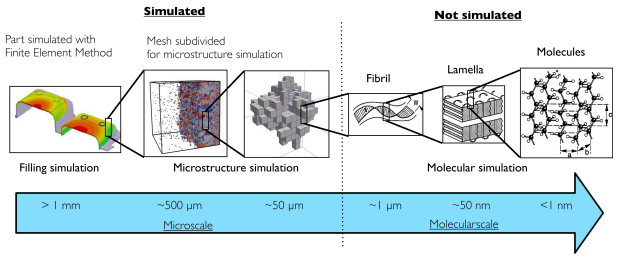

Figure 1: Macro-Micro level

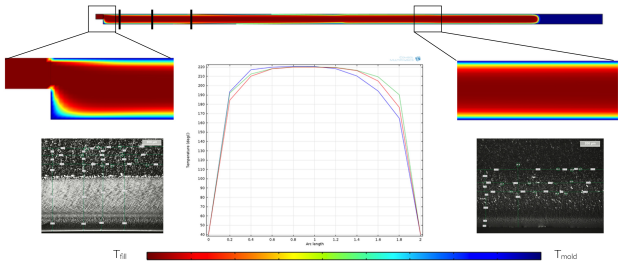

Figure 2: Flow results

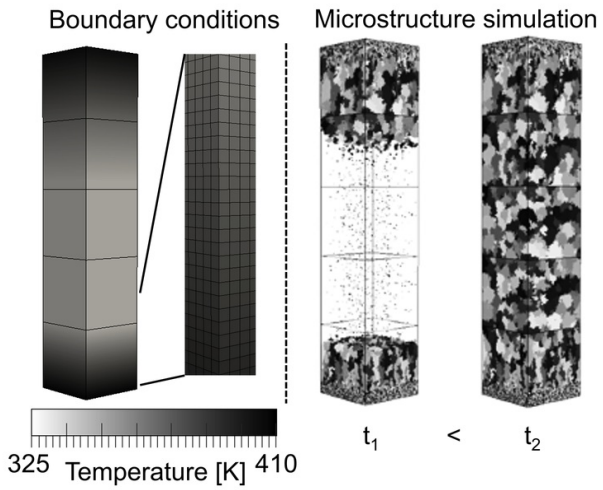

Figure 3: Miscrostructure simulation