Seminar im Rahmen des GRK 2078

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Datum:	Mo., 09.07.2018
Uhrzeit:	14:00h
Ort:	Geb. 10.23, 3. OG (R 308.1 – KM-Seminarraum)
Titel:	**Multiscale simulation of an injection molded polypropylene part and derivation of its microstructure dependent elastic and thermal properties**

Abstract

Industrial plastic parts, made of semi-crystalline polymers, are often produced by injection molding. In this process the melt undergoes a complex deformation and cooling history which results in an inhomogeneous distribution of spherulites in the component. The different size and shape of the spherulites induce local variations of the mechanical and thermal properties in the final part. To evaluate these inhomogeneities in an isotactic polypropylene (α-iPP) component accurately, a 3D multi-scale, integrated simulation approach has been developed. At first, a coupled mold filling, heat transfer and solidification analysis is achieved at the macro-scale and the predicted velocity and temperature fields are transferred to the micromodel. Based on a calculation of the Gibbs free energy, with thermal, athermal and flow induced contributions, nucleation probabilities are calculated on a Representative Volume Element (RVE) at the microscale and converted to phase changes. The subsequent growth process is computed via a path integration of the crystal growth front. Thus, the evolution of the spherulitic microstructure during the crystallization process is predicted. To evaluate their effective mechanical and thermal properties a dedicated two-level homogenization scheme has been developed. It consists firstly to derive, at the nano-scale, the effective properties of the lamella build of crystalline and amorphous phases. In this study, not only the radial growing lamella of amorphous and crystalline phases is homogenized, but also its “cross hatched” lamellar structure by introducing an appropriate lamella design. Moreover, molecular dynamic simulations have been performed in order to derive unknown crystalline and amorphous phase properties, like their respective Hooke matrix. At the micro-scale, the spherulite microstructure is homogenized via a 3D radial distribution of equivalent lamellae around its mono-crystal center. Finally, the application of the developed homogenization scheme allows the prediction of the distribution of effective mechanical and thermal properties over the component thickness in different sections of a staggered α-iPP plate, produced by injection molding.

References

[1] G. Laschet, M. Spekowius, R. Spina, Ch. Hopmann: „Multiscale simulation to predict microstructure dependent effective elastic properties of an injection molded polypropylene component“, Mechanics of Materials, vol. 105, pp. 123-137, 2017.

[2] G: Laschet, M. Apel, J. Wipperfürth, C. Hopmann, M. Spekowius, R. Spina: „Effective thermal properties of an isotactic polypropylene (a-iPP) injection moulded part by a multiscale approach”, Materialwissenschaft und Werkstofftechnik, vol. 48, pp. 1213-19, 2017.

[3] M. Spekowius, R. Spina, C. Hopmann: “Mesoscale simulation of the solidification process in injection molded parts”, J Polymer Engineering, vol. 36 (6), pp. 563-574, 2016.

Alle Interessenten sind herzlich eingeladen.

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