A finite strain, thermo-mechanically coupled material model for semi-crystalline polymers, incorporating crystallisation kinetics

S. Felder*[1], H. Holthusen[1], S. Hesseler[2], F. Pohlkemper[2], J.-W. Simon[1], T. Gries[2] and S. Reese[1]

[1] Institute of Applied Mechanics (IFAM)
RWTH Aachen University
Mies-van-der-Rohe-Str. 1, 52074 Aachen, Germany
e-mail: sebastian.felder@rwth-aachen.de, web page: https://www.ifam.rwth-aachen.de

[2] Institut für Textiltechnik (ITA)
RWTH Aachen University
Otto-Blumenthal-Straße 1, 52074 Aachen, Germany
web page: https://www.ita.rwth-aachen.de

ABSTRACT

Thermoplastic polymers are an important class of materials for many technically relevant applications. In contrast to thermosets, which form irreversible chemical bonds, they can be repeatedly reshaped after heating above the melting point. As a consequence, they are well-suited for forming processes. A specific class of thermoplastics are semi-crystalline polymers, which partly crystallise after cooling from the melt. During the forming process, a complex interplay between crystallisation and the formation of residual stresses arises. In order to avoid cost- and time-consuming trial and error approaches, a strong demand for computational models, which accurately predict the material and structural response of the part during forming, emerges.

To this end, a phenomenological material model is presented in this work. The thermo-mechanically coupled constitutive framework is derived in a thermodynamically consistent manner and valid for large deformation, as well as large deformation rates. In order to account for the amorphous and crystalline regions of the underlying microstructure, a rule of mixture of the energy contributions of both phases is applied, which is in line with [1]. For this purpose, the overall degree of crystallinity serves as an input parameter, which is depending on the temperature history and modelled by means of a non-isothermal representation of the Avrami equation [2].

To model the crystalline regime, a hyperelastic-plastic constitutive framework is derived, which is in line with [3, 4]. To account for the spring back effect after forming, isotropic and nonlinear kinematic hardening of Armstrong-Frederick type are incorporated. The amorphous phase is modelled by means of a visco-hyperelastic material formulation based on the work of Reese and Govindjee [5]. As a result, this work represents an important step towards the accurate and efficient prediction of the complex rate, temperature and degree of crystallinity depending material behaviour of semi-crystalline polymers.

REFERENCES

[1] N. Dusunceli and O. U. Colak, “Modelling effects of degree of crystallinity on mechanical behavior of semicrystalline polymers”, *Int. J. Plasticity*, **24**, 1224-1242 (2008).

[2] K. Nakamura, K. Katayaama and T. Amano, “Some aspects of non-isothermal crystallization of polymers. II. consideration of the isokinetic condition”, *J. Appl. Polym. Sci.*, **17**, 1031-1041 (1973).

[3] I. Vladimirov, M. Pietryga and S. Reese, “On the modelling of non-linear kinematic hardening at finite strains with application to springback - Comparison of time integration algorithms”, *Int. J. Numer. Meth. Eng.*, **75**, 1-28 (2008).

[4] T. Brepols, I. Vladimirov and S. Reese, “Numerical comparison of isotropic hypo- and hyperelastic-based plasticity models with application to industrial forming processes”, *Int. J. Plasticity*, **63**, 18-46 (2014).

[5] S. Reese and S. Govindjee, “A theory of finite viscoelasticity and numerical aspects”, *Int. J. Solids Struct.*, **35**, 3455-3482 (1998).