Towards a multi-scale modelling methodology for biobased polymer fibre composites

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ABSTRACT

Within the framework of the Horizon 2020 project “BIO4SELF” on fully biobased polymer fibre composites a multi-scale modelling methodology will be implemented to connect manufacturing conditions with material parameters, polymer dynamics and product properties. The scheme aims to design macroscale processing conditions for the fibre spinning and composite fabrication process, meso-scale morphology as well as micro-scale molecular structure to achieve ultimately desired mechanical properties.

Atomistic-scale molecular dynamics (MD), phase-field as well as continuum kinetics, and micromechanical modelling including classical laminate theory as Materials Relations (MR) will be coupled to have a multi-scale modelling applied to phenomena at broad time- and length-scales. The atomistic molecular dynamics modelling results relate to the properties of the pure polymer phases and are linked to the phase-field and continuum modelling via characteristic material parameters or functions. For example, the molecular mobility and time-scale dependence on molar-mass distribution and temperature will be taken into account for the phase-field models of polymer crystal morphology evolution.

The mechanical properties of two-phase composite materials consisting of reinforcement fibres embedded in a polymer matrix are typically calculated by continuum micromechanical models. The models are written up for representative volume elements in the materials and this includes geometrical parameters for the composition (e.g. fibre content and orientation) and material parameters (e.g. crystal structure, strength, stiffness of both phases). Such micromechanical models have been validated for short fibre composites manufactured by injection moulding and compression moulding. For fabric based composites, classical laminate theory is used for materials relations together with the determined elastic constants of single plies.