DFG-Project Schm-746/74-2

Improved toughness/stiffness balance of nanoparticle filled polyamide composites – simulation supported property/morphology correlation

Begin of the project: 01.02.2013
Estimated end of the project: 28.02.2015

Project goal

A hierarchical modelling concept is developed on the basis of a multi-phase polyamide (PA6) in order to improve the toughness balance by establishing a suitable morphology (Fig 1). In a three-phase material system, a polyether soft phase and nano scale layered silicates (Montmorillionite, MMT) increase the mechanical properties e.g. material toughness (impact resistance) and material stiffness (Young's modulus).

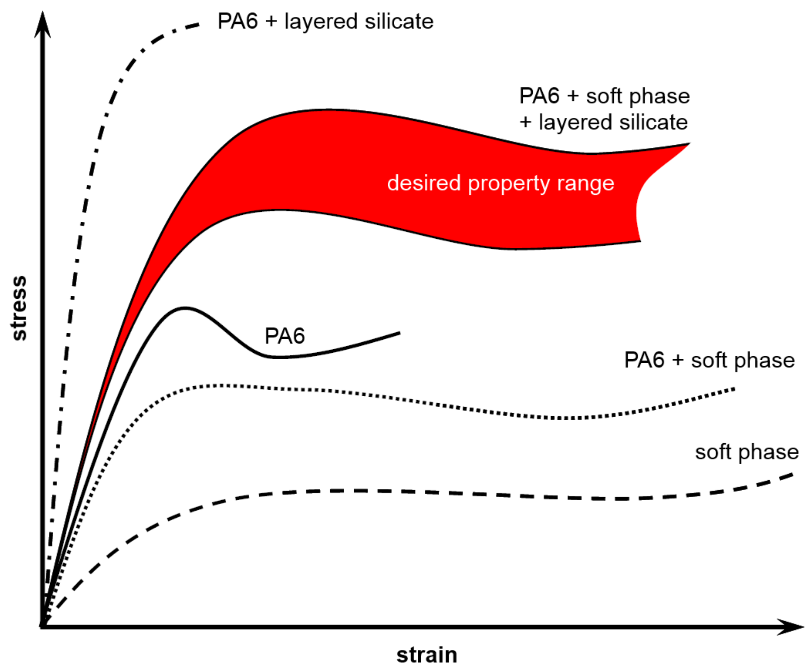

Fig 1: Schematic overview of the 'desired' material properties through the simulation supported structure-properties correlation.

Methodology

In the first part of the project heterogeneous Finite-Element (FE)-Models are constructed on the basis of experimental results of real microstructures. Firstly, the individual influence of the soft phase and layered silicates is studied. Subsequently, their combined influence is investigated. In the second part of the project the constructed FE-Model is used to investigate mechanical properties depending on the phase size, phase fraction and crystallographic orientation of individual material phases. In addition, matrix phase coupling, boundary surface morphology and voids of microscopic size are taken into account for the investigation of the structure-properties relation.

The matrix delamination is modelled by cohesive zone method (CZM) in FEM. The basic parameters of the CZM, which originate from the traction-separation law, are the critical stress and the fracture energy. In the case of matrix delamination from the layered silicate, both parameters are derived from MD simulations.

On the atomistic scale the compound under investigation is represented through a ternary material system, namely PA6, the silicate layer and, due to manufacturing, an organic modifier. Upon the creation of the initial structure and several relaxation runs, nano-tensile and nano-shear tests (Fig 2) with different strain/shear rates at several temperatures are performed to calculate critical stresses and the surface binding energy between PA6 matrix and the layered silicate.

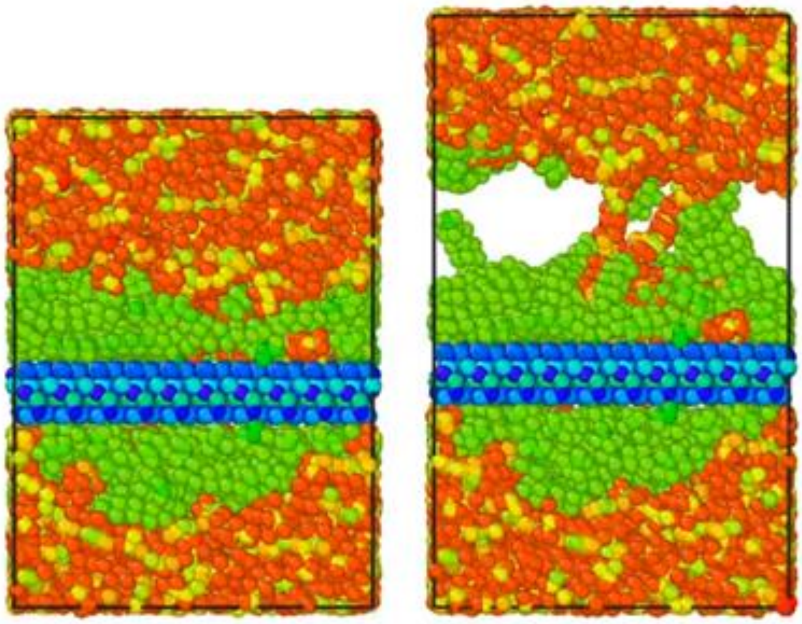

Fig 2: Nano tensile test. Blue: layered silicate, green: organic modifier, red/yellow: PA6.

Partners

This project will be done in collaboration with the Institute of Polymer Technology (IKT) at the University of Stuttgart. At the IKT, the experimental research of structure-properties relation will be performed. In addition, specimens with desired material properties will be manufactured within the scope of the joint project.

Acknowledgement

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Contact Person

Dipl.-Ing. Jing Wiedmaier
Institute for Material Testing, Material Science and Strength of Materials (IMWF)
University of Stuttgart
Pfaffenwaldring 32
70569 Stuttgart
Tel.: +49 / 711 685-64378
E-Mail: Jing.Wiedmaier@imwf.uni-stuttgart.de

Dipl.-Ing. Wolfgang Verestek
Institute for Material Testing, Material Science and Strength of Materials (IMWF)
University of Stuttgart
Pfaffenwaldring 32
70569 Stuttgart
Tel.: +49 / 711 685-62583
E-Mail: wolfgang.verestek@imwf.uni-stuttgart.de