DFG-Projekt Schm 746/74-1

Improved toughness–balance of nano-particle-filled polyamid-composite – simulation- supported properties/morphology correlation

Begin of Project: 01.12.2008
End of Project: 30.09.2011

Aim

On the basis of an example of multi-phasic polyamids, a hierarchial modelling concept will be developed in order to improve the toughness-balance by finding a suitable morphology like the optimal phase-size, -fraction and -orientation, by structuring, by matrix-phase-coupling, boundary surface morphology and micro voids (Figure 1). Important is the implementation of a polyether-soft phase as well as nano scale layered silicates (Montmorillonit) in order to increase the toughness (impact resistance) and stiffness (E-Module). As a central point of the modelling technique is the construction of heterogeneous Finite-Element (FE)-Models, which consider the semi-crystalline polyamid matrix and the dispersed soft-phases as well as the nanoparticles into account for calculations.

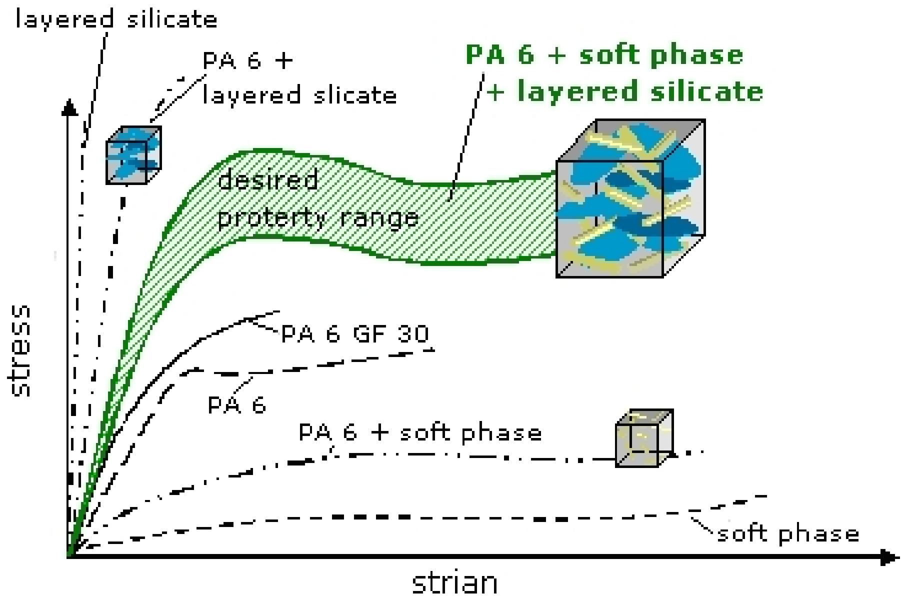

Fig 1: Schematical overview of the 'desired' material properties through simulation supported correlation of properties and morphology.

Methodology

The project is divided into two parts. In Part-I of the project, on the basis of experimental results the real micro-structures under the influence of the soft-phase and the layered silicate must be modelled, first separately and then together. In Part II of the project, micro-structures that have been improved due to virtual change in the toughness and stiffness must be simulated, conceptualised and in the end, tested experimentally. The characterization of morphology and mechanical characteristics provide the input data for the corresponding simulations. On their basis, virtual morphology with a free variation of form, fraction and distribution of the dispersed phases would be generated and improved taking into account the modelled mechanical behaviour.

In this way, the micro-structure model simulated with the help of FEM would be finally verified through experiments and thus its applicability verified. The results of the calculations from the simulations are applied for the conceptualization and the production of real material morphologies with improved characteristics. As main mechanical parameters, the Izod-ductility according to ISO 180, the area under the stress-strain curve got from the tension tests and the E-Module according to ISO 178 at room-temperature are defined at IKT. Furthermore, the insitu local strains are measured with the help of photogrammetry.

Recent Results

In this study semi crystalline nylon 6 and copolymer particle-modified Nylon 6 are investigated. The aim of this paper is to show how micro-mechanical modelling can predict their elastic behaviour from the experimentally observed morphology.

Semi crystalline nylon 6 is an important structural material. Characterisation and prediction of their mechanical behaviours is indispensable to enable their wide use. Semi crystalline Nylon 6 has aspherulitic morphology, consisting of a radial assembly of amorphous layers and nano-sized crystalline lamellae (Fig. 1). The mechanical properties are strongly dependent on the crystallinity and the crystalline orientation. To simulate the overall mechanical properties of the semi crystalline nylon 6, it is desirable to know the properties of each component (amorphous layers and crystalline lamellae). The Young's modulus of the amorphous matrix has been determined by a nano indentation. Unfortunately, because of the size of the individual lamellar crystals, it is realistically not possible to get the information of the crystalline lamellae from experiment. The elastic property of the crystalline lamella could be given by an inverse modelling with a self-consistent embedded cell model. The model idealises the micro-structure to consist of an amorphous matrix with randomly arranged crystalline lamellae as embedded reinforcing fibres. In this model, a rectangular lamella is surrounded by an amorphous matrix, which is again embedded in the semi-crystalline nylon 6 with the mechanical behaviour to be determined iteratively in a self-consistent manner (Fig. 2). The Young's Modulus of nylon 6 can been calculated by an appropriate integration of results of all lamellae orientations.

Recent investigations have shown that the toughness of semi-crystalline nylon 6 can be improved by dispersion of additional second-phase elastomer particles. The Young's Modulus of this nylon 6/ copolymer composite is predicted by embedded cell models in conjunction with the finite element method. A circular elastomer inclusion is surrounded by the nylon 6 polymer matrix, which is again embedded in the composite.

In both cases we calculated the elastic properties of two isotropic polymers at ambient temperature for very small deformations (0.05-0.25%). It means, the viscoelastic behaviour, even a viscoelasto-plastic behaviour should not be considered. Good agreement is obtained between experiment and the prediction with the self-consistent embedded cell models.

In the final stage, the elastic properties of the composite containing both type of particles, is numerically predicted with a parametric study in order to find an optimised composition with respect to the mechanical material properties.

Partners

This project will be done in collaboration with the Institute for Plastics (synthetic, organic, processed materials) Engineering (IKT), Stuttgart. At the IKT, the experimental research of morphology as well as of mechanical characteristics will be done along with the production of real material morphologies with improved characteristics.

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Contact Person

Dipl.-Ing. Jing Huang

Tel.: +49 / 711 685-67674
Fax: +49 / 711 685-62635
E-Mail: jing.huang@mpa.uni-stuttgart.de

Dipl.-Ing. Simon Geier

Tel.: +49 / 711 685-62661
Fax: +49 / 711 685-62066
E-Mail: simon.geier@ikt.uni-stuttgart.de