Multi-Scale Modeling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance

Reporting

Project Information

NANOMODEL

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Project website

Project closed

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Coordinated by
BASF SE
Germany

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Final Report Summary - NANOMODEL (Multi-Scale Modeling of Nano-Structured Polymeric Materials: From Chemistry to Materials Performance)

Executive Summary:
The FP7 project NanoModel - Multi-Scale Modeling of Nano-Structured Polymeric materials: From Chemistry to Materials Performance (Grant Agreement number: 211778) has finished smoothly in accord with the planning as outlined in Annex I to the Grant Agreement. There were no fundamental structural changes necessary. The goal - the sustainable development of validated multiscale modeling methods and tools for rational nanocomposite design- has been reached. This involved synthesis, modeling method development, validation and to a certain extent the development of new materials. The focus of the project was on understanding, design and performance of nanocomposites consisting of surface modified nanoparticles(NP) embedded in technically relevant polymer matrices. In particular, silica, hematite, barium titanate and yttrium europium vanadate particles embedded in polystyrene (PS), poly(methyl methacrylate) (PMMA), poly(butylene terephthalate) (PBT) and polyamide (PA66) were synthesized, characterized, dispersed, characterized again, tested and simulated on length scales from atomistic simulation to constitutive modelling by finite element methods (FEM). To this end, it was necessary to combine expertise from synthesis, testing, processing and simulation (both method developers and application scientists). To ensure sustainability of simulation methods developed, important method developments were integrated into a commercially available modelling software system. To facilitate fruitful collaboration among and across expert areas, the project consisted of three layers -basic method & software development, model systems preparation with characterization and testing and the validation against each other. The concept was successful due to a vivid exchange within and between the three layers.
In a comparative study, the different approaches mentioned above, were validated. It was shown, by direct comparison with neutron scattering results, that the applied simulation strategies describe the structure of the nanocomposites well. New synthesis approaches were developed to create very well defined and characterized nanocomposites with fully dispersed nanoparticles. In detailed analysis, the ordering of the polymer around the nanoparticle could be described, and also the dynamics. The dynamics of free polymer chains in the vicinity of the NP is slowed down both in grafted and ungrafted samples, which has consequences for the processing. Also, reasonable estimates of the mechanical performance together

could be obtained and rationalized. Rules for successful stable dispersion of surface modified nanoparticles in polymer matrices could be developed, which is important for commercialization. In our systems, no specific "nano-effect" boosting the mechanical performance of nanocomposites could be detected. Under regular conditions relevant for industrial usage, we could not find extraordinary performance of composites filled with nanoparticles compared to conventional fillers. Thus, since the materials properties of nanocomposites generated throughout the project did not show interesting new effects leading to new application, it was not justified to file any patent. This is, however, consistent with the fact that nanocomposites commercially still do not play a role as materials. The toolbox developed and validated in this project, however, is not restricted to these systems. Since they are available in a commercial package, the tools will be applied in the future to further promising concepts for development of light weight performance materials. In particular the newly developed MD-FEM coupling scheme and the Fti-MC method are important steps towards a rational materials development, since they allow for modelling and simulation of complex materials with high chemical detail.
The project was by its nature multidisciplinary, involving chemists, physicists, mathematicians, chemical and mechanical engineers and software developers from industry and academia. 12 publications are meanwhile published, more than 60 presentations were given, 2 publications are submitted and 6 in preparation. The MD-FEM coupling development is transferred to a DFG SPP project (1369) for further development. There was intensive collaboration among the young team consisting of 13 PhD students (among them 2 females), 10 Postdocs (2 females), 3 Diploma theses students and 2 undergraduates from 11 countries.

Related documents

final1-data-extract-specific-publishable-summaries-december-2012-part-4-attachments-2011-12-23-211778-1076746-final-publishable-report.pdf

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