FLAG-ERA

Joint Transnational Call 2017

GraSage: Modelling of the electrical and thermal transport mechanisms in graphene nano-modified polymer compounds and fibres

Main area: BSR06_Modelling charge and heat transport in GRM - based composites
Keywords: Compounds; Composites; Fibres; Melt-spinning; Polymer; Graphene; Modelling
Duration (months): 36
Total project funding: € 792.680

Abstract

Graphene, the two-dimensional allotrope of carbon, has benefited from tremendous research activities in the field of composite materials as highlighted by countless published studies focusing on graphene-modified nano-composite materials like compounds and fibres. However, no qualitative and quantitative model of the interactions between graphene and the surrounding matrix material is currently available. This lack of knowledge about structural formation of composite material does impede the development of high-performance graphene-modified fibre materials. Thus, the main goal of the “GraSage” project is to develop a model describing the orientation and structural interaction of graphene within a surrounding polymer matrix during a fibre melt-spinning process able to predict the electrical- and thermal properties of the nanocomposites.When CNTs and carbon black are combined with a polymer matrix, the spinning conditions have great influence on the orientation of nano-materials in a fibre matrix leading to different mechanical, thermal and electrical properties. Such effects are not yet quantified when graphene is used. Consequently, an experi-mental study on graphene-modified polymeric compounds and fibres will be performed. The parameters to be modified are the aspect ratio of graphene, the mass concentration of graphene in the polymer, the ma-trix polymer itself, the number of capillary dies in the melt-spinning process, the length-to-diameter ratio of the capillary dies, mesh configuration of spin filters and finally the melt draw ratio as well as the applied solid-state draw ratio. The obtained fibres will be characterized with respect to their structural, mechanical, thermal and electrical properties.Parallel to the experimental study, the melt-spinning process of the nanocomposites will be simulated at the nano- and microscales to provide an in-depth view of the structure and thermo-electrical properties of the polymer/graphene interface. These predictions obtained at small scales will then be transferred to a macro-scopic quantitative model based on neuronal nets and fuzzy logics to finally obtain the electrical and thermal properties of a graphene-reinforced polymeric compound- and fibre.This project will result in a multiscale qualitative- as well as quantitative understanding of the thermal and electrical properties of graphene modified polymer matrices. The state of the art will be overcome significantly; furthermore, the obtained knowledge will strengthen the technology transfer of graphene composites from lab- to industrial scale thanks to the availability of tailor-made composite- and fibre products. The fundamental knowledge acquired in this project will serve as a basis to reduce research efforts and product development in the field of graphene-modified nano engineered polymer composites.

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