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Project title: Modelling of electrical and thermal transport mechanisms in graphene-modified polymer compounds and fibres (GraSage)

Partners: Maastricht University, KU Leuven, AITEX

Run-time: 01.09.2018 – 31.08.2020

Conveyor: Deutsche Forschungsgemeinschaft

Mission Statement

Graphene, a two-dimensional allotrope of carbon, has been and still is the subject of enormous research efforts in the field of nanocomposite materials, as numerous publications have shown. However, neither qualitative nor quantitative models of the interactions between graphene and the surrounding polymer matrix are currently available. Ignorance of the structural formation in nanocomposites prevents the development of cost-efficient yet high-performance graphene-modified fibre materials. The aim of the project "GraSage" is therefore the modelling of graphene-modified nanocomposite materials to improve their electrical, thermal and mechanical properties. Understanding the underlying mechanisms accelerates technology transfer from laboratory to industrial scale through the availability of bespoke composite and fibre materials and the associated reduction in research effort and product development time. This will strengthen Europe's position in the field of graphene research through high-quality patents and publications, as well as the position of graphene manufacturing and processing companies in the marketplace.

Solution Path

In a statistical experimental design, graphene-modified polymer composite fibres are prepared by melt spinning, with parameters such as the aspect ratio and mass concentration of graphene, the type of polymer matrix, the number and length-to-diameter ratio of the capillary nozzles in the melt spinning process, the grid geometry of the spin filters, and the melt and solids draw rate be varied. The resulting fibres are examined for their electrical, thermal and mechanical properties. In parallel, the nano- and microscopic nanocomposite fabrication processes are simulated by a molecular dynamic approach to provide detailed insights into the structure and thermoelectric properties at the polymer-graphene interfaces. A quantitative model is created for predicting the influence of process conditions on the resulting material properties. This model is refined using experimental data and serves as the basis for future composite and fibre fabrication processes.

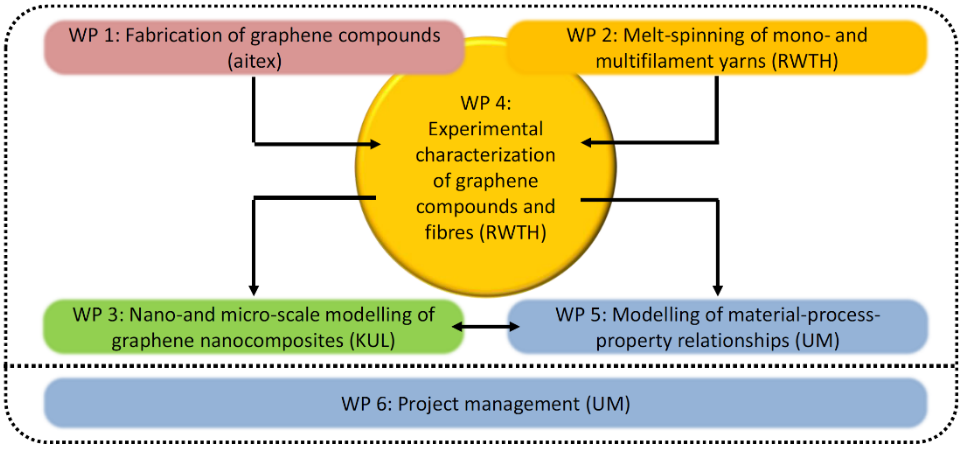

Fig. 1: Project overview

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