Current projects within the DPI programme Performance Polymers

Project #805: *Probing interfacial damage in composites with mechanofluorescence (INTERMECHANOPOL)*
Eindhoven University of Technology (NL)
December 2017 - November 2021

Project leaders: Prof. Rint Sijbesma, Dr. Hans Heuts
Researcher: Annelore Aerts (PhD)

Obtaining information about the stresses in the interfacial region on a molecular level would be beneficial for the optimization of the properties of polymer nanocomposites. This project now aims to develop a method for the optical detection of these stresses and this method will be based on mechanochemical principles. Mechanosensitive fluorescent probes will be developed and employed to investigate the relation between interfacial interaction strength and mechanical properties.

Project #806: *2D material coatings for fibres (2D4CF)*
The University of Manchester (UK)
September 2017 - March 2021

Project leaders: Prof. Robert Young, Dr. Mark Bissett
Researcher: Jingwen Chu (PhD)

This project will aim to exploit the unique strain-sensitive behaviour of various 2D materials to coat reinforcing fibres typically used in composite materials, and then use Raman spectroscopy to measure the strain present at the interface between the reinforcing fibre and the polymer matrix in which it is embedded. The interfacial strength between the 2D material, the reinforcing fibre, and the polymer matrix will also be tuned through modification of the surface chemistry. The 2D materials that will initially be the focus of this research will include graphene, hexagonal boron nitride (hBN), and several transition metal dichalcogenides.

Project #811t17: *Reliable Prediction of Residual Structural Integrity and Damage- Evolution During Long-Term Fatigue in Thermoplastic Composites (SafeRide)*
[a] University of Twente (NL), [b] Delft University of Technology (NL)
September 2018- August 2022

Project leaders:
[a] Prof. Leon Govaert, Dr. Martin van Drongelen
[b] Prof. Bert Sluys, Dr. Frans van der Meer
Researchers:
[a] Bharath Sundararajan (PhD)
[b] Dragan Kovacevic (PhD)

The long-term performance of thermoplastic composites (for automotive and aerospace) is currently very poorly predictable. As a consequence, composite parts are generally overdesigned and, therefore, not optimal in weight reduction. Safe-Ride aims at developing a new predictive design tool that improves the predictability of part performance substantially. The multiscale predictive model will be developed in a hybrid experimental/numerical approach with an extensive experimental programme for characterization and validation.

Project #812t17: ***Physics-based fatigue design tool for matrix cracking and delamination in unidirectional and sandwich composites under multi-axial fatigue loads with arbitrary R-ratio : development, validation and finite element implementation (FATHOM)*****;**

Ghent University (BE)
December 2018- November 2022

Project leader: Prof. Wim van Paepegem
Researchers: Dr. Mohammad Kajikazemi (PostDoc), Josef Sommer (PhD)

A physics-based fatigue design tool for matrix cracking and delamination in unidirectional and unidirectional tape based laminates under multi-axial fatigue loads with arbitrary R-ratio is developed in this project. The models rely on variational stress analysis and a very limited set of physical parameters. Their analytical basis makes them appropriate for fast assessment in a finite element environment, leading to an industrially applicable design tool. The application to sandwich composites will be included. The modelling framework has the potential to be extended in future for other physical degradation mechanisms such as temperature, moisture, defects and gas/liquid diffusion.

Project #819: ***Controlling electrical percolation in hybrid thermoplastic composites through informed selection of fillers (HPC)***
The University of Manchester (UK)
October 2018 - September 2022

Project leaders: Prof. Ian Kinloch, Dr. Mark Bissett, Prof. William Sampson
Researchers: Kailing Lin (PhD), Yubao Deng (PhD)

Carbon black-filled thermoplastics are used for applications where electrical conductivity is required. However, carbon black's low aspect ratio means that a high loading is needed to establish conductivity, causing processing issues. The recent commercialisation of graphene and nanotubes brings the opportunity to use a new generation of high aspect ratio fillers. We have shown previously that such fillers behave synergistically for mechanical properties and we will transfer this knowledge to conductive applications. In particular, we will develop a detailed understanding of the processing-structure-property interdependence of these fillers using in-situ, ex-situ and modelling techniques, to predict their behaviour in industrial applications.

Project #820: ***Microstructure-based Modelling of the Intrinsic Kinetics of Aging and Deformation of Polymer Glasses (MIKADOGLAS)***
Eindhoven University of Technology (NL)
September 2018 – August 2019

Project leaders: Prof. Patrick Anderson, Dr. Markus Hutter, Dr. Lambèrt van Breemen
Researcher: Dr. Georgios Vogiatzis (PostDoc)

Extension of a previous PP project which developed innovative methodology allowing the molecular simulations of physical ageing of polymeric glasses solely based on their atomistic structure and chemistry. The principal focus of the extended project would be the elucidation of structure-property relations from first principles, i.e. starting from chemistry till the prediction of mechanical properties; thereby synthetic chemists are provided with design rules for producing materials with improved performance.

Project #822: Processing for Enhanced Product Performance (PEPP-3)

Eindhoven University of Technology (NL)
June 2019 – June 2020

Project leaders: Prof. Leon Govaert, Dr. Hans van Dommelen
Researcher: Dr. Ahmad Amiri Rad (PostDoc)

Extension of current PP project that developed anisotropic viscoelastic-viscoplastic macro-mechanical model, which is able to capture the orientation and rate-dependent response of short-fibre reinforced polymers. The model was implemented in a commercial finite element framework. The current project will further improve the predictability of this model via incorporating appropriate criteria to predict plasticity controlled and crack-growth controlled failure.

Project #823: Modular, designer polydopamine adhesives for facile and versatile surface conjugation of function to polymers (PODOPAD)
University of Twente (NL)
June 2019 - May 2023

Project leaders: Prof. Julius Vancso, Dr. Joost Duvigneau, Dr. Mark Hempenius
Researcher: Roland Milatz (PhD)

Bio-inspired, versatile surface-anchoring phenolic-based macromolecular adhesives (polydopamines) will be developed exhibiting dual functions. The polymers allow surface anchoring to various hard-to-bond substrate polymers (by spraying, dip-coating, and gradient-coating) and enable subsequent coupling of functional layers. These layers include (1) antifouling polyzwitterionic brushes, and (2) fluorescent, covalently coupled coatings for greenhouse films. Attachment of functional groups will be achieved by click chemistry and surface-initiated ATRP.

Project #824: Micromechanical modelling of complex composite systems for improved failure prediction and product design (Micro-Tough)
Eindhoven University of Technology (NL)
June 2019 – May 2023

Project leaders: Prof. Leon Govaert, Dr. Tom Engels, Dr. Lambert van Breemen
Researcher: Martijn Wismans (PhD)

To keep pace with the speed of modern-day innovation, predictive engineering is the key tool to enable the required speed. This is more than true for reinforced engineering-thermoplastics that are increasingly used to light-weight design by replacing metal. Ideally, a full in-silico design and optimization of parts is performed and only a final ‘real-life’ validation test is required. Reality is that current tools are still far from quantitative, requiring multiple design and testing iterations, and material modifications. This project aims at developing micromechanical tools that bring higher accuracy to current design tools and increased speed to material development cycles.

Project #825: Development of Hyperpolarized and 1H Fast MAS NMR Spectroscopy for the study of performance polymers (HYPERFAST)
Radboud University (NL)
June 2019 – May 2023

Project leader: Prof. Arno Kentgens
Researcher: 1 PhD

Solid-state nuclear magnetic resonance (ssNMR) spectroscopy allows the investigation of structure and dynamics of polymers relating to their functional behaviour. NMR probes the local environment of a nucleus without relying on their crystalline arrangement. The main objective of this proposal is to capitalize on two important methodological developments that can remedy shortcomings of NMR for studying complex polymer systems. We intend to develop Ultrafast magic angle spinning (MAS) NMR combined with sophisticated rf pulse schemes for high resolution NMR of protons in the solid-state. Furthermore, we aim to optimize and extend Dynamic Nuclear Polarization (DNP) methodology for the study of low gamma nuclei in polymeric systems relevant in a DPI context.

Project #826: Multi-layered wear-resistant coatings with additional functionality – new strategies for enhancing the tribological performance of polymers in demanding environments (MERCURIAL)
Polymer Competence Centre Leoben (AT)
September 2019 – September 2022

Project leaders: Priv.-Doz. Dr. Sandra Schlögl, Dr. Andreas Hausberger, Prof. Wolfgang Kern
Researcher: 1 PhD (+1 PhD if proof of concept is realized).

In MERCURIAL the next generation of wear-resistant coatings for polymers is developed to replace light-metals with conventionally and additively manufactured polymers by: (i) minimized friction and wear rate under dry/lubricated conditions, (ii) self-adaptation to the counter-body's surface topography and self-healing after overloading, (iii) increasing functionality by introducing gradients and (iv) cost-efficiency by high-rate, large-area, vacuum-chamber-free atmospheric pressure plasma deposition. The versatility of the developed materials/processes will allow for the coating of numerous polymers (particularly thermoplastics) due to low-temperature deposition. Performance versus morphology/function will be studied in detail to understand mechanisms for high wear-resistance/long-term stability of functional coatings in demanding environments.

Project #827: Impact modelling of polymers: high-rate experiments for solid-state simulations (IMPRESS)
[a] University of Oxford (UK), [b] University of Nottingham (UK)
October 2019 – April 2023

Project leaders:
[a] Prof. Clive Siviour
[b] Dr. Davide De Focatiis
Researchers: 2 PhDs and 2 PostDocs

Polymers and composites are often used in products exposed to impact events; e.g. car bumpers, mobile phone cases or bike helmets. However, their behaviour during impact is not well understood, which prevents us from optimising the material properties and structural design. The final products are therefore heavier or less effective than they could be. This project will develop new methods for measuring the response of polymers to impact, and for modelling and designing polymer structures. In *the future, it will allow us to produce high performance, recyclable, polymers that are optimised to work efficiently in different impact applications.*

Project #828: Elastomer DEgradation under MEchanical Loading: investigation of coupling effect (EDEMEL)
[a] Ecole Nationale Supérieure d'Arts et Métiers Paris (FR), [b] IFREMER Institute (FR)
March 2019 – March 2022

Project leaders:
[b] Dr. Pierre-Yves le Gac
[a] Prof. Bruno Fayolle
Researchers: 1 PhD and 1 PostDoc (1.5 years)

Polymer degradation is one of the major topics when considering enhancement of service life of structures. In order to consider lifetime prediction of polymers, studies are generally performed considering only mechanical loading, such as fatigue, or only chemical degradation, such as oxidation, in terms of mechanisms and kinetics. However, in service, polymers are subjected to both mechanical loading and chemical degradation. This project, with a step by step approach, will investigate the strong coupling effects between chemical degradation of elastomers and mechanical loading (static and dynamic) with the aim to propose more reliable lifetime predictions.

Project #829: Physical and chemical ageing of amorphous polymers by molecular simulation (PEARL)
[a] Eindhoven University of Technology (NL), [b] National Technical University of Athens (Greece)
July 2019 – June 2023

Project leaders:
[a] Prof. Patrick Anderson, Dr. Markus Hütter, Dr. Lambert van Breemen
[b] Prof. Doros Theodorou
Researcher: 1 PhD and 1 PostDoc (3 years)

A combination of simulation methods will provide molecular-level insight into the parallel ageing mechanisms of amorphous polymers, specifically quantifying the effect of physical ageing and chemical degradation by UV irradiation and oxidizing agents on the response to deformation of glassy polymers, and determining the effect of deformation on the diffusion pathways and diffusivity of penetrant molecules.