Current portfolio of the DPI program Performance Polymers PP

Project #805: Probing interfacial damage in composites with mechanofluorescence (INTERMECHANOPOL), 1 PhD
December 2017 - November 2021

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 #811t17: Reliable Prediction of Residual Structural Integrity and Damage- Evolution During Long-Term Fatigue in Thermoplastic Composites (SafeRide), 2 PhDs
September 2018- August 2022

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 program 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). 1 PhD and 1 PostDoc
December 2018- November 2022

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), 2 PhDs
October 2018- September 2022

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 #823: Modular, designer polydopamine adhesives for facile and versatile surface conjugation of function to polymers (PODOPAD), 1 PhD
June 2019 - May 2023

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), 1 PhD
June 2019 – May 2023

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), 1 PostDoc
October 2021 – June 2024

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), 2 PhDs
September 2019 – August 2022

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), 2 PhDs and 2 PostDocs
October 2019 – September 2023

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), 1 PhD and 1 PostDoc
Ecole Nationale Supérieure d'Arts et Métiers Paris (France) and IFREMER Institute (France)
March 2020 – February 2023

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), 1 PhD and 1 PostDoc
November 2019 – October 2023

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.

Project #837: Linking rheological material functions to polymer crystallization (RHECRY), 1 PhD and 1 PostDoc
March 2021 – August 2024

Flow-induced crystallization in polymers is a fundamental problem in both polymer science and industrial processing. It is related to the ability of polymer segments to orient and nucleate. Despite the enormous progress to date by means of experiments and simulations, the link between the underlying nonlinear rheology of polymers and their crystallization properties is still missing. We aim at providing the ingredients for this link:
we propose a multi-scale approach combining state-of-the-art nonlinear shear experiments and atomistic simulations and constitutive modeling in order to correlate rheology, undercooling and material parameters with the degree of crystallization in model and commercial polymers.

Project #838: Supramolecular modulation of the network connectivity in vitrimers (SUPRAMOD), 1 PhD
November 2020 – October 2023

Converting thermoplastics into vitrimers via reactive processing is a promising approach to upcycling processing scraps and post-consumer waste. However, the constant, temperature-independent network connectivity of vitrimers represents a formidable processing challenge. Vitrimers with high crosslinking densities typically exhibit high viscosities, which precludes injection moulding. Furthermore, in the welding of vitrimer components, there is an inherent trade-off between weld reversibility and strength. We propose to overcome this obstacle by integrating supramolecular additives ("supramods") that thermally modulate the degree of network connectivity. This approach will enable crosslinked materials to truly behave as thermoplastics at processing temperatures.

Project #839: Dynamic chemistry for tunable reversible bonding in bulk and at interfaces (DYNABOND), 1 PostDoc
March 2021 – March 2024

This project aims to develop new reversible chemistry for dynamic covalent polymer networks and controllable interfacial adhesion based on abundant and cheap components that are already widely in use in commercial polymers. Transesterification of phosphate esters will be investigated in elastomers with the aim to develop materials with better bonding to fillers and improved recyclability; they will be investigated in thermoplastics to enhance mechanical stability. Reversible bonding between thiols or alcohols and cyclic anhydrides at interfaces will be used to develop interfacial bonding with a high control over bonding level using a combination of thermal and oxidative triggers.

Project #840: Engineering the rheology ANd processinG-induced structural anisotropy of poLymEr composites with non-Brownian fibrous particles (ANGLE), 1 PhD
March 2021 – February 2025

Reinforcing polymers with glass fibers is essential to reach strength and stiffness while maintaining light-weight. However, the improvement in ultimate properties is highly dependent on the microstructure of the fiber reinforcements and its anisotropy. This microstructure is developed during processing in the molten state and is governed by the interplay between flow and geometrical parameters, polymer rheology and particle characteristics. We will perform an experimental-numerical study on processing of polymer-fiber composites, putting particular emphasis on unravelling the effects of geometrical confinement, polymer viscoelasticity and interactions with spherical particles. Thereto, sophisticated in-house developed rheometers and numerical codes will be used.

Project #841: Understanding the Rheological Origin of Striped Flow Marks in Injection Molding (UROSFMIM), 1 PhD and 1 PostDoc
March 2021 – February 2025

Striped flow marks are one of the most serious defects in injection molding, affecting the appearance and mechanical properties of plastic products. Despite much effort from academia and industry, no consensus has been reached on critical occurring conditions and mechanisms.

In this project, we will clarify the rheological origin of striped flow marks by constructing an instability diagram for injection molding. Model polymer blends will be used to reveal the start of flow instability by tracking the spatiotemporal deformation and orientation of domains using off-line and on-line methods with supports from simulation on the flow pattern of polymer blends.

Project #843: Recyclable high-performance composites with reversible interface bonding (RECOMP), 1 PhD
January 2021 – January 2025

Composite recycling is a challenge, especially if the full material value is to be retained. In this project we will expand reversible bonding concept to aramid fibre and fibre mesh composites. We aim to design systems with strong, but "reversible interfaces" between fibres and polymer matrix by utilizing reversible bonding between the two components. Previously the reversible bonds were mainly designed to exist between matrix components only. This will lead to superior interfacial properties at the same time as the re-processability is enhanced or the bonding can be reversed to recycle the composite back to high-quality fibres and matrix components.

Project #844: Modelling and Design of Multiphase Polymeric Materials for High Performance Applications Across Multiple Scales (MuMPol), 1 PhD and 1 PostDoc
November 2020 – October 2024

The project will develop an integrated simulation chain for the sorption and transport properties of high performance, multiphase materials, such as semi crystalline polymers or nanocomposites for challenging industrial applications. A Molecular Dynamics (MD) simulation of the phases will be bridged with macroscopic methods in a hierarchical approach adopting key material parameters and producing structure-property correlations useful to guide the design and the optimization of such materials, as well as to reduce the number of experimental tests required. A comprehensive, dedicated experimental campaign will be designed and performed to validate and integrate the simulation approach.

Project #845: A joint molecular modelling and experimental approach to developing novel thin-film polymer barriers for gas containment systems (DINGOES), 1 PhD
October 2020 – October 2023

In the short to medium term future it is likely that hydrogen powered vehicles will use lightweight compressed hydrogen gas storage tanks made from plastic and fibre-reinforced composite materials. To reduce the gradual leakage of gas from such reservoirs it is intended to develop thin barrier films using interfacial synthesis methods. A pre-screening of candidate polymers will first be carried out using molecular modelling techniques in order to reduce costly syntheses of the real materials.

Project #850: Mechanism of Electrical Aging Caused by Different Structural Defects in Performance Polymer Materials (MEAPP), 2 PhDs and 1 PostDoc
September 2021 – September 2025

The booming of global electric vehicles and electronic industries creates an increasing demand for qualified performance polymers used for related insulation components. However, defects in these materials will initiate electrical aging and breakdown gradually, raising potential and realistic safety issues. This project aims to unravel *the mechanism of surface/bulk electrical aging induced by different structural defects inevitably remaining in performance polymers used, under typical electric fields as well as electric fields coupled with heat and humidity similar to actual applications; and develop an optimal interpretable electrical aging model via machine learning techniques based on backpropagation, dropout and homogeneity pursuit algorithms.*

Project #851: Creep Fatigue Interaction in Performance Polymers at High Temperatures (CreepFat), 1 PostDoc
October 2021 – September 2024

The project deals with the characterisation of the fatigue behaviour of short fibre reinforced (sfr) performance polymers and the fatigue life calculation of cyclically loaded parts in a closed simulation chain outgoing from the injection moulding process to fatigue failure. In this work we want to specifically characterize the creep – fatigue interaction at high temperatures for sfr performance polymers and implement the derived viscoelastic models in the existing simulation chain. Moreover, we want to capture the effect of possible local degradation under high temperature service conditions on lifetime under static and fatigue loads.

Project #852: Thermo-electrical ageing mechanisms in polymer-ceramic nanocomposites for energy storage applications (TEAMs), 1 PhD and 1 PostDoc
January 2022 - January 2025

Various polymer-ceramic nanocomposites have been developed in recent years for energy storage applications. Such materials are of significant scientific and industrial interest because they combine high breakdown strength and dielectric permittivity thereby potentially increasing energy storage in comparison with the materials traditionally used as dielectric media in capacitors. Such application also requires an acceptable service lifetime but despite numerous studies, understanding of their electro-thermal ageing mechanisms is still lacking. This study aims to establish a theoretical framework for the electro-thermal ageing processes in polymer-ceramic nanocomposites and to develop a new ageing model, which can be used for lifetime predictions.

Project #853: Polyamides/Glass fiber recycling by reactive extrusion, 1 PostDoc
January 2022 – January 2024

The objective is to develop performing materials from chemical recycling of Polyamides PA filled with Glass Fibres using the reactive extrusion process. The driving idea is to reduce the viscosity of the PA by chemical modification in order to limit the breakup of glass fibres while in situ synthesis an organic crosslinked phase in order to regenerate the polyamide/glass fibres interphase. The study aims to go from the fundamental aspects of the reaction/structuration to the scaling-up of the reactive extrusion process.

Project #854: Monitoring lifetime of thermoplastic composites by combining analytics and machine learning (TRAIL), 1 PhD
January 2022 – January 2025

We explore ways to combine two non-destructive monitoring methods to monitor long fibre reinforced composite with semi-crystalline polymer matrix. We test oriented carbon composite with single orientation direction and other materials. We use data based modelling to find out whether we can monitor crack formation and crack *propagation using specific electrical characterizations (particularly impedance based) first when assisted by direct structural data from X-ray based methods and subsequently without direct structural information. The ultimate goal is to use these ideas to estimate the remaining useful lifetime in composite structures.*