

PhD Project

PO-STRETCHED: Molecular modelling of stretch-induced crystallization in polyethylene and polypropylene layers

Project description:

A PhD position in the *Theory of Polymers and Soft Matter Group* at the Eindhoven University of Technology is available with funding from the Dutch Polymer Institute (DPI), <https://www.polymers.nl>, an industry-driven international collaboration platform for pre-competitive research in the field of polymers. Within the **PO-stretched** project we aim at developing a multiscale molecular approach to provide insight into the morphology and properties of two industrially relevant systems, being

- monolayer and bilayer polyethylene (PE) films;
- polypropylene (PP)-based composites,

and the influence of mechanical stretching. Using a chain-of-knowledge approach, the emphasis will be on rational materials design using atomistic simulations and statistical theory. Parameters will be extracted from simulation for use in continuum models of the initial stages of crystallization, deformation, and fracture in a scale-bridging sense. The extremely large amount of experimental data that exists needs an explanation, therefore we run the **PO-stretched** project in collaboration with industrial DPI partners, including Sibur, Dow and Borealis. The commitment of industrial consultants of DPI to help develop the necessary connection with experimental testing are proof of immediate industrial relevance and guarantee direct and efficient transfer of knowledge between parties involved.

Aim of the PhD project:

In the **PO-stretched** project we undertake **multiscale simulations of semi-crystalline morphology development** upon high-strain mechanical deformation of polyethylene and polypropylene to understand the mechanisms controlling crystallization, toughness, permeability, determine optimization design strategies and provide a molecular basis for finite-element simulations. In parallel, the kinetic effects that dominate the crystallization of polymers are going to be investigated using analytical approaches developed in Eindhoven, and extended for the polymers in strongly confined geometries. Analytical approaches are to be developed to explain the fracture behaviour and determine fracture toughness values of the relevant polymer composites.

Qualifications of applicant:

Talented, enthusiastic candidates with strong simulational skills holding a university degree (M.Sc.) in (Theoretical) Physics, Mechanical Engineering, Materials Science, Scientific Computing, or a closely related discipline are encouraged to apply. Preferably, the candidate has been exposed to any of these topics: statistical physics, computer simulation methods, and polymer physics. Proficiency in the C++ programming language is an advantage. Good knowledge of spoken and written English is an essential asset.

Appointment details:

We offer a full-time, four-year PhD position at a dynamic and ambitious university, with an immediate starting date. The project will be carried out at the Theory of Polymers and Soft Matter group at the Department of Applied Physics, Eindhoven University of Technology, the Netherlands. The candidate will collaborate closely with the Dutch Polymer Institute and its partners. More information about this PhD position can be obtained from dr. Alexey Lyulin a.v.lyulin@tue.nl, tel. +31 (0) 40-247-4253. Application documents (pdf only) should be sent by email, including a letter of application, a short description of scientific/work experience, a full curriculum vitae, transcripts of B.Sc. and M.Sc. degrees, and contact information of two potential referees.