

**MULTISCALE MECHANICS OF POLYMERS AND POLYMER
COMPOSITES
TRACK NUMBER 300 - MULTISCALE AND MULTIPHYSICS
SYSTEMS**

F. DETREZ¹, J. A. W. van DOMMELEN², S. PFALLER³ AND A. STRACHAN⁴

¹ Université Paris-Est, Laboratoire de Modélisation et Simulation Multi Echelle, UMR 8208 CNRS
5 Boulevard Descartes, 77454 Marne-la-Vallée Cedex 2, France
fabrice.detrez@u-pem.fr

² Department of Mechanical Engineering, Eindhoven University of Technology
5600 MB Eindhoven, PO Box 513, The Netherland
j.a.w.v.dommelen@tue.nl

³ Lehrstuhl für Technische Mechanik, Friedrich-Alexander-Universität
Egerlandstraße 5, D-91058 Erlangen, Germany
sebastian.pfaller@fau.de

⁴School of Materials Engineering and Birck Nanotechnology Center, Purdue University
West Lafayette, Indiana 47907, United States
strachan@purdue.edu

Key words: Multiscale modelling, Polymer, Nanocomposite, Numerical homogenization, Atomistic-continuum coupling methods

ABSTRACT

Polymers and their composites feature many physical mechanisms that operate over an immense range of length and time scales, which are very often coupled. The integration of these mechanisms poses significant challenges to the scientific community that requires sophisticated multiscale models and experiments.

This mini-symposium will highlight the recent theoretical, computational, experimental, and combined approaches that address (a) structure-property relations as well as (b) the multi-physics coupling of mechanics with, *e.g.*, chemical reactions, phase transformation, biological processes, and electromagnetic fields, or quantification of uncertainties across scales and physics.

Possible topics include (not exclusive list):

- Materials: (3D) bulk polymers, *e.g.* thermosets, thermoplastics, elastomers, gels, liquid crystal elastomers, composites, nanocomposites, bioinspired materials; (2D) polymer membranes, graphene; (1D) fibres, muscle fibres, carbon nanotubes.
- State and its evolution during processing: molten state or solid state (both semi-crystalline or

glassy amorphous polymers), and the effects of processing including polymerization, curing and crystallization.

- Properties: viscoelasticity, plasticity, damage, creep, fracture, adhesion, instability.
- Multi-physics coupling: piezo-elasticity, electro-elasticity, magneto elasticity, flexo-elasticity, photo-elasticity, magneto rheology, crystallization, effect of physical aging and chemical degradation on mechanical behaviour.
- Interfacial phenomena: surface effects, interfaces, interphases, confinement effects.
- Simulation techniques: *ab initio*, molecular dynamics, FEM, FFT, numerical homogenization, atomistic-continuum coupling methods (sequential, coupling, hierarchical methods, domain-decomposition methods), phase field methods, data-driven methods, topology optimization.

With regard to engineering applications, the following fields are of interest, but are not limited to:

- Additive manufacturing, 3D-printing
- Composites and nanocomposites for the aviation, aerospace, automotive, and pneumatic industries
- In-situ sensors for *e.g.* damage detection, moisture measurement, matrix-filler delamination detection
- Smart materials and sensors
- Energy storage, *e.g.* membrane lithium ion batteries
- Long-term performance in engineering applications
- Influence of processing conditions and production methods
- Design of biomimetic materials
- Soft-matter design for food and cosmetics
- Recycling of polymers, sustainable polymers