

DPI Annual Meeting

13 and 14 November 2018

Holiday Inn, Eindhoven, the Netherlands









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 **DPI**
The Polymer
Research Platform









19 DPI
Achievements and recognitions
DPI Publications 2011-15
PhD Theses 2011-15
D Awards DPI awards Glasgow airport
at Glasgow's Business Conference 2015
Dr. Barbara Shuter, PhD Fellow awarded 2015
"Entrepreneurial Game Award" in 2015

19 DPI
Welcome

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19 DPI







DPI

2018: Highlights - 1
Scientific achievements and recognitions

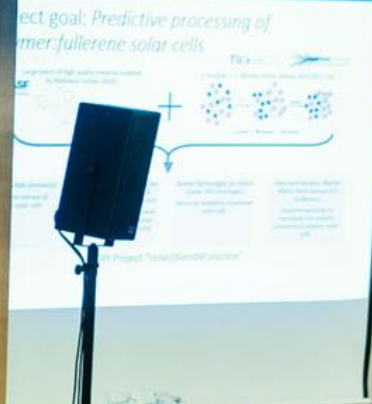
- Number of DPI Publications (2017): 70
- Number of PhD Theses (2017): 10
- GRACM PhD Award for DPI postdoc Georgios Vogiatzis
- DPI to again co-organize Conference in 2019
- Fellow DPI secretaries: "New Psephology" Conference, "Cold Neurophysiology"

Why polymer solar cells?

- Potential to be made cheap ("print like a newspaper")
- Increasing efficiencies through increasing understanding



Project goal: Predictive processing of polymer:fullerene solar cells





Institute for Energy Technology

Energy Technology)

ment)

TU/e

DPI

Design Process Institute

ety

number of wafers per day





A presentation slide with a blue background and a white rectangular area containing text. The TU/e logo is in the top right corner. The title is 'Adjustable nanoporous polymers Based on smectic liquid crystals'. Below the title, the speaker's name 'Dirk Jan Mulder' and the date '13 November DPI Annual Meeting 2018' are listed.

TU/e
EINDHOVEN
UNIVERSITY OF
TECHNOLOGY

Adjustable nanoporous polymers Based on smectic liquid crystals

Dirk Jan Mulder

13 November
DPI Annual Meeting 2018





The Energy - Water Challenge



Nanoporous liquid crystal networks



Proton conductivity



MICROSCALE SIMULATIONS OF THE MECHANICS OF SPONGY-PARTICLE SYSTEMS

Monica Zakhari, Markus Hütter, Patrick Anderson

TU/e

















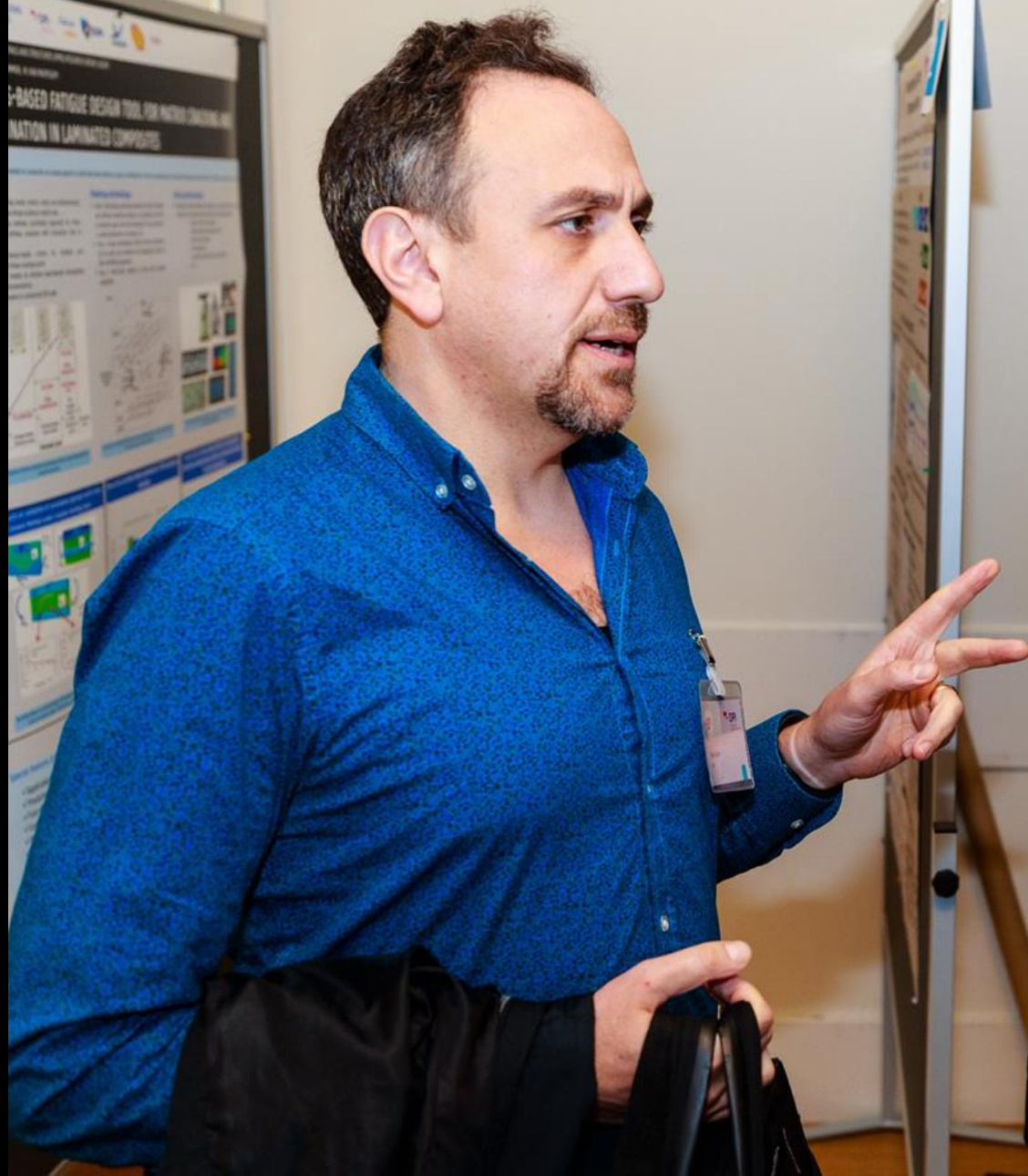
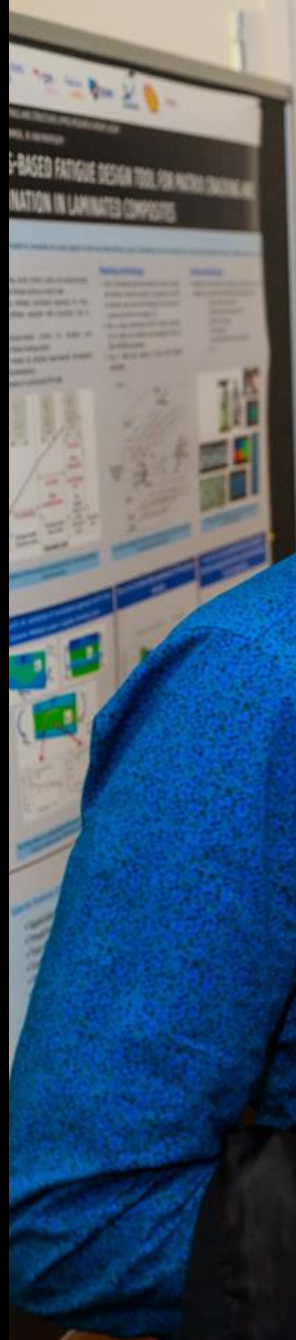




















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Lifetime prediction of DPI

DPI Safe-Mode

Reliable prediction of lifetime based on the safe-mode operation of DPI. SafeMode aims at developing an early prediction model for DPI lifetime.

Background

- Lightweight DPI are widely used in various applications.
- Performance under varying conditions are not easily predictable during development.
- Hence, it is necessary to study the failure modes of DPI under various conditions.



Fig. 1. DPI structure.

Research objectives

- Characterize the DPI under various conditions.
- Develop a predictive model for DPI lifetime.

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DPI

NWO
Netherlands Organisation
for Scientific ResearchTU/e
Technische Universiteit
Eindhoven
University of Technology

Programmable helical twisting in oriented bilayer films

by Rob Verpaalen

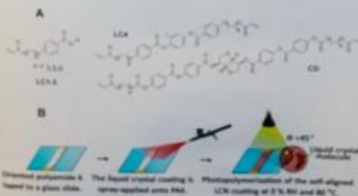
dr. M.G. Debije, dr. ing. C.W.M. Bastiaansen, dr. ir. T.A.P. Engels

Introduction

In a continuous search for novel, high-end products, traditional commodity polymers form an interesting class of materials to introduce new functionalities. The existing industrial infrastructures should preferably undergo only minor changes to extend their range of application, as for example in stimuli-responsive, smart textiles and soft robotics. Here, a low impact, though elegant, method is employed in which a liquid crystal network (LCN) coating is spray-applied onto stretched and extremely humidity-sensitive polyamide 6 (PA6) films. The films demonstrate helical twisting as a chiral dopant was added to the liquid crystal (LC) mixture, eliminating the need to cut films at an angle.

Materials and Methods

A 4 μm LC coating was spray-applied onto a commercially available oriented PA6 film (15 μm) to prepare humidity-sensitive bilayer actuators (Scheme 1). The LCs (LC1-4) were copolymerized after UV-initiated cleavage of the initiator to form a LCN. A helical twist in the bilayer is created by the addition of a small amount of a right-handed chiral dopant (CD).



Scheme 1. A. The photopolymerizable liquid crystals LC1-4 and chiral dopant CD. B. Bilayer preparation procedure.

Reference

R. C. P. Verpaalen, *J. Mater. Chem. A*, 2016, 17724-17729

SFD / Stimuli-responsive functional materials and devices

The humidity response of 20 \times actuators were investigated in humidity chamber into which the (see Figure 1). Theta, θ , relative throughout the thickness of the



Figure 1: Programmed actuators at various humidity levels and viewing angles.

Conclusion

We have demonstrated the possibility of creating humidity-sensitive bilayer actuators by spray-coating a liquid crystal network onto a polyamide 6 film.









2D Material Coatings for Fibres

Jingwen Chu, Prof. Robert J. Young, Dr. Mark A. Bissett
The University of Manchester

MANCHESTER
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Digital Polymer

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Introduction

Due to its excellent mechanical properties, carbon nanotube (CNT) and graphene have been widely used in various applications. The same technique can be employed for some high-performance fibres, such as para-aramid fibres and carbon fibres, and some other 2D materials like MoS₂.

Previous research has investigated the carbon nanotube (CNT) fibre (just to name a few) and carbon fibre composites for strain-sensing with the help of these materials. This technology can be further expanded to produce other 2D materials.

Other papers for the mechanical view of TMDs show changes in their electronic properties under strain to be detected by photoluminescence.

Objectives

- Coat reinforcing fibres with a selection of 2D materials and characterise using a variety of analytical techniques.
- Tune the strain sensitivity of 2D materials through improvement of the coating formula as well as method and through chemical modification of the strain reporters.
- Embed coated fibres into an epoxy resin matrix and report the strain performance.
- Measure and compare the mechanical properties of composites reinforced with coated and un-coated fibres.
- Investigate the optoelectronic properties of TMDs coated fibres and the effect of strain on the electronic structure.

Sample Preparation

Coating solution: 2D materials, Electrochemically-reduced graphene (EG)

Fibres (Kevlar, glass and carbon fibres)

Coating solution: High-purity epoxy resin and 2D coating (EG or graphene)

Dip Coating

Dry at 100 °C for 24 h (fully remove NMP and cure the resin)

Results

Figure 1: Comparison of the Raman 2D band shift rates (cm⁻¹/%) for three types of fibres coated with electrochemically-reduced graphene and GO graphene (average of 8 measurements for each).

Electrode material	Graphene	Carbon fibre	Glass fibre
EG	-3.3 ± 0.3	3.7 ± 0.7	-3.5 ± 0.7
GO	-5.0 ± 1.2	4.3 ± 1.2	-7.5 ± 0.8

Figure 2: Representative Raman 2D shift with strain for EG coated onto glass fibre (in (a) before and (b) after being embedded in the epoxy resin matrix).

Figure 3: Representative Raman 2D shift with strain for EG coated onto glass fibre (in (a) before and (b) after being embedded in the epoxy resin matrix).

Future Work

Investigate the optoelectronic properties of TMDs coated fibres and the effect of strain on the electronic structure.



Invited speakers

- Dr. Søren Bøwadt (European Commission)
- Dr. Just Jansz (Expertise Beyond Borders)
- Prof. Kim Ragaert (University of Ghent)
- Dr. Patricia Vangheluwe (PlasticsEurope)



Plastics in the circular economy

Industry needs to embrace the circular economy in the wake of growing public concern on plastic waste

Dr. Just Jansz
Expertise Beyond Borders BV

DPI Annual Meeting, Eindhoven
13 November 2018







Marine plastic litter: 8 countries in Asia account for 75% of plastic waste washed into the oceans



- India, despite its 1.3bn people, falls outside the top ten thanks to armies of rag pickers, although this statistic is being challenged
- Only China could afford Western-style waste management in the near future



We





A lot of plastics is used only once



Global plastics production and use, 1950-2015

Millions tons

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Plastics 2030: A Necessary Commitment for a Plastics Circular Economy

Dr. Patricia Vangheem
Director Consumer & Environmental Affairs

DPI Annual
12 November

PlasticsEurope
Association of Plastics Manufacturers



Plastics 2030 – Voluntary Commitment for a Plastics
Circular Economy

Dr. Patricia Vangheluwe
Director Consumer & Environment

DPI Annual Event
13 November 2018

PlasticsEurope
Association of Plastics Manufacturers



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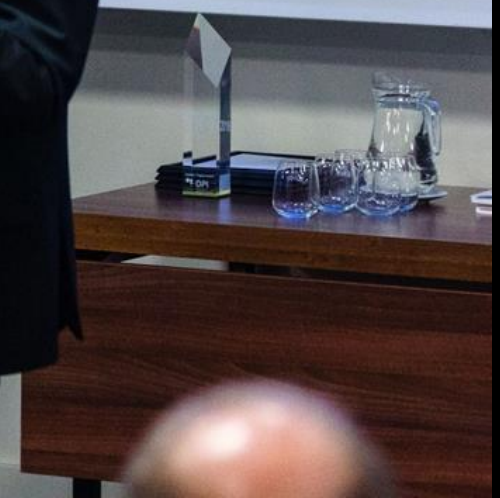
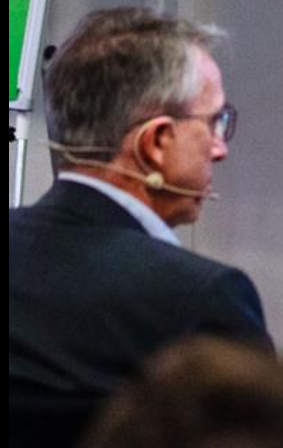
FACULTY OF ENGINEERING
AND ARCHITECTURE

TO RECYCLE OR NOT TO RECYCLE

IT'S HARDLY A QUESTION

Prof. Kim Ragaert

Annual Meeting - Eindhoven, November 13th 2018



BASIC PRINCIPLES OF MECHANICAL RECYCLING




BASIC PRINCIPLES OF MECHANICAL RECYCLING



- Compounding
- Twin screw extrusion
 - Melt filtration
 - Adequate feeding, venting...

- Conversion (as virgin)
- Extrusion (cast or film)
 - thermoforming
 - Injection moulding
 - ...



A woman with blonde hair tied back, wearing a purple blazer and a black top, stands at a podium. She is wearing a headset microphone and looking towards the right. Behind her is a large projection screen displaying a slide. The slide features a background image of a large pile of colorful, shredded plastic waste in shades of blue, purple, and green. A white rectangular box is overlaid on the center of the screen, containing text. The text reads: "Materials Science & Polymer Engineering are the key to improved and increased mechanical recycling of polymers".

Materials Science & Polymer Engineering
are the key to improved and increased
mechanical recycling of polymers







Towards a Circular Economy for Plastics

Søren Bowadt
DG Research & Innovation
European Commission







The workhorse material of our current economy entails urgent environmental, social and economic drawbacks



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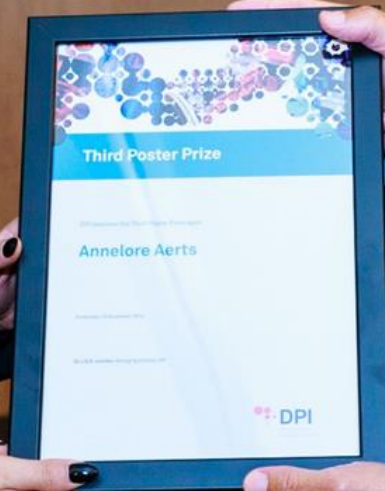


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Dynamische
Platform

Golden Thesis Award
Awarded to
Dirk Jan Mulder
for his thesis
on
DPI

Thesis Award
Awarded to
Hans van Peltz
for his thesis
on
DPI





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First Poster Prize

DPI Organizes the First Poster Prize each year

Hanne van der Kooij

Department of Chemistry

Utrecht University

For more information, please contact:

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Jeroen Jansen
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Second Poster Prize

DPI bestows the Second Poster Prize upon

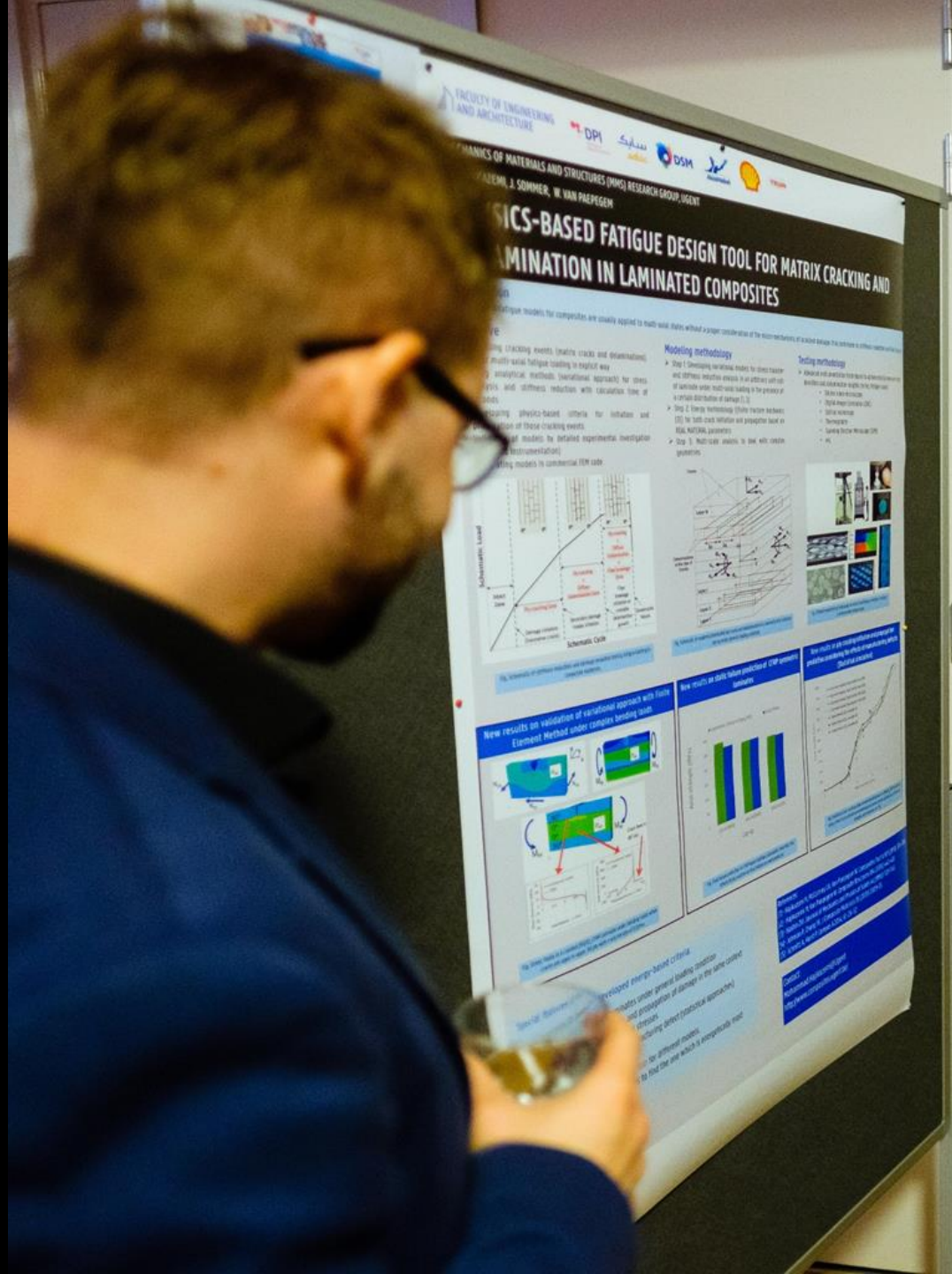
Rob Verpaalen

Recipient: 11 November 2018

By: S.A. van der Vliet, Managing Director







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MECHANICS OF MATERIALS AND STRUCTURES (MMS) RESEARCH GROUP, UOEA
SADEGH, J. SOMMER, W. VAN PAEPGEN

PHYSICS-BASED FATIGUE DESIGN TOOL FOR MATRIX CRACKING AND DELAMINATION IN LAMINATED COMPOSITES

Fatigue models for composites are usually applied to multi-scale plates without a proper consideration of the micro-mechanics of crack damage. This lecture is devoted to the development of a multi-scale fatigue design tool for matrix cracking and delamination in laminated composites. The tool is based on a physics-based approach for stress analysis and stiffness reduction with calculation time of minutes. The tool is based on a physics-based criteria for initiation and propagation of those cracking events. The tool is validated against experimental investigation (instrumentation) and existing models in commercial FEM code.

Modeling methodology

- Step 1: Developing variational models for stress transfer and stiffness reduction process in an arbitrary laminate under multi-scale loading in the presence of a periodic distribution of damage. (1, 2)
- Step 2: Energy minimization (variational mechanics) for both crack initiation and propagation based on REAL MATERIAL LAAMIERS.
- Step 3: Multi-scale models to deal with loading conditions.

Tooling methodology

- Developed multi-scale tool for stress transfer and stiffness reduction process in an arbitrary laminate under multi-scale loading in the presence of a periodic distribution of damage. (1, 2)
- Step 1: Variational mechanics
- Step 2: Energy minimization (variational mechanics)
- Step 3: Multi-scale models to deal with loading conditions

Micro-mechanics Level

Schematic Cycle

New results on validation of variational approach with finite Element Method under complex loading conditions

New results on multi-scale prediction of GFRP laminates

References

1. Sadegh, J., Sommer, W. & Van Paepgen, W. (2015) A multi-scale fatigue design tool for matrix cracking and delamination in laminated composites. *Journal of Applied Mechanics*, 82(10), 101001.
2. Sadegh, J., Sommer, W. & Van Paepgen, W. (2016) A multi-scale fatigue design tool for matrix cracking and delamination in laminated composites. *Journal of Applied Mechanics*, 83(10), 101001.

Contact: Sadegh@uoea.edu.iq
<http://www.mms.uoea.edu.iq>



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SADEGH, J. SOMMER, W. VAN PAEPGEN

Pursuing the Next Frontier: Structure and Dynamics

Structure and Dynamics

References

1. Sadegh, J., Sommer, W. & Van Paepgen, W. (2015) A multi-scale fatigue design tool for matrix cracking and delamination in laminated composites. *Journal of Applied Mechanics*, 82(10), 101001.
2. Sadegh, J., Sommer, W. & Van Paepgen, W. (2016) A multi-scale fatigue design tool for matrix cracking and delamination in laminated composites. *Journal of Applied Mechanics*, 83(10), 101001.

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Programmable helical twisting in oriented bilayer films

Dr. Rob Verpaalen

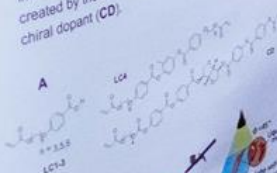
Dr. M.G. Debijs, Dr. Ing. C.W.M. Bastiaansen, Dr. Ir. T.A.P. Engels

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Materials and Methods

A 4 μm LC coating was spray-applied onto a commercially available oriented PA6 film (15 μm) to prepare humidity-sensitive bilayer actuators (Scheme 1). The LCs (LC1-4) were copolymerized after UV-initiated cleavage of the initiator to form a LCN. A helical twist in the bilayer is created by the addition of a small amount of a right-handed chiral dopant (CD).



The humidity response of 20 x 2 x 2.078 mm bilayer actuators were investigated in a temperature-controlled humidity chamber into which dry or humid nitrogen was fed (see Figure 1). Theta₀ refers to the in-plane twist angle throughout the thickness of the coating.



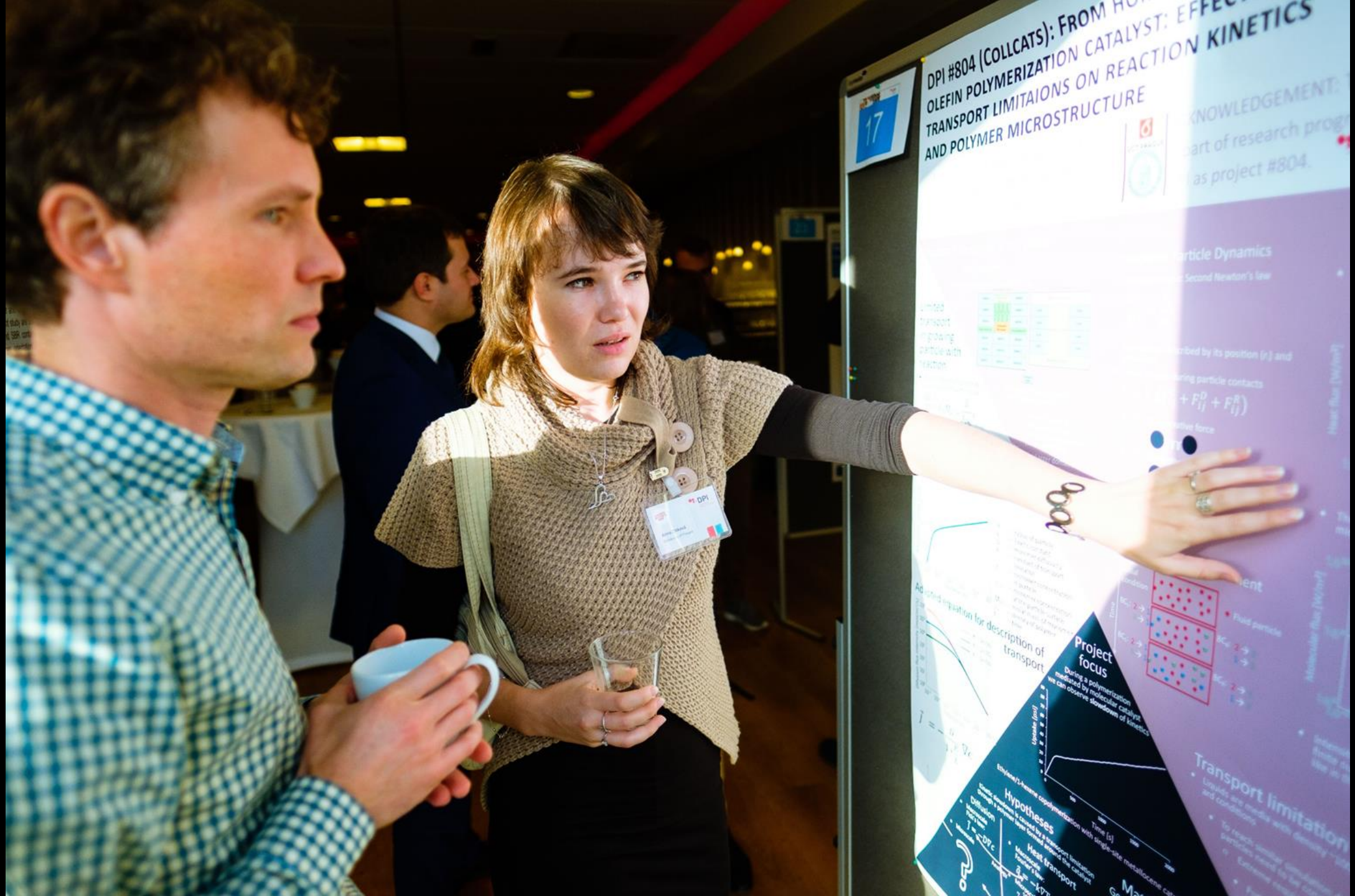
Figure 1. Programmable humidity-sensitive bilayer actuators at various humidity levels.

Conclusion and Outlook
We show that an elegant spraying method can be employed to program helical twisting in bilayer actuators. The bilayer actuators can be used to create programmable actuators with a wide range of applications. In principle, any other stimuli-responsive LC mixture can be used to create helical twisting and to introduce a different twist angle by changing the concentration of the chiral dopant.

Acknowledgments
This research was part of the research program of SFB 121/1713-202.

Reference

R. C. P. Verpaalen, J. Mater. Chem. A, 2018, 6, 17724-17728



DPI #804 (COLLCATS): FROM HOLES TO PARTICLES: EFFECTIVE TRANSPORT LIMITATIONS ON REACTION KINETICS AND POLYMER MICROSTRUCTURE



KNOWLEDGEMENT: part of research program as project #804.

Particle Dynamics

Second Newton's law

described by its position (r) and

including particle contacts

$$m \ddot{r} = -\nabla U(r) + F_{ij}^D + F_{ij}^R$$

Force



Project focus

During a polymerization mediated by molecular catalyst we can observe slowdown of kinetics

Hypotheses

Diffusion limitation

Mass transport limitation

Heat transport limitation

Transport limitation

Unlikely are readily with density $\sim 10^2$

To reach similar simulation particles need to be far apart

Extreme model

















Service Institute for Industrial Analytics

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Cast film extruded IPP studied by SAXS/WAXS/RAMAN

Erico di Sacco^{1,2}, Giuseppe Portale^{1,2}

¹Materials, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands
²U.S.O. Box 902, 5600 AX Eindhoven, The Netherlands

Motivation/Aim

Cast an isotactic polypropylene (IPP), processed via cast film extrusion, undergoing during the casting process. Small angle X-ray scattering is the most powerful tool to record highly detailed structural information. In this work, SAXS/WAXS/RAMAN spectroscopy is thus combined here to study the conformational state of the polymer chains during the casting process.

Machine parameters: $T_{\text{extr}} = 230^{\circ}\text{C}$; $T_{\text{cool}} = 15^{\circ}\text{C}$; high mesophase content; $T_{\text{meas}} = 20^{\circ}\text{C}$. After casting, the mesophase will tend to convert to the more stable alpha phase, followed by the beta phase.

Structure of the mesophase (France) using a setup that allow simultaneous acquisition of data (see photo).

Results: mesophase melted at a certain T_{m} and then water-cooled to the desired temperature. The structure of the mesophase is determined using a certain method.

Analysis

Analysis of the mesophase structure using SAXS/WAXS/RAMAN.

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Computational Modeling of Propene Polymerization

Giuseppe Portale

Department of Chemical Sciences, University of Groningen, 3000 SB Groningen, The Netherlands

Propene polymerization is a highly complex process. In this work, we present a computational study of the reaction mechanism for propene polymerization. The reaction mechanism is studied using a combination of experimental and computational data. The reaction mechanism is studied using a combination of experimental and computational data.

Low-Coverage Model (LCM) is a model of the reaction mechanism. The model is based on the reaction mechanism of the reaction between the active species and the monomer. The model is based on the reaction mechanism of the reaction between the active species and the monomer.



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Quantitative Structure - Activity Relationships in Metallocene-Based Olefin Polymerization

On the connection of stereoselectivity, regioselectivity and molecular weight in *rac*-bis(2-Me-4-Fl indenyl)ZrCl₂ type catalysts

C. Dine, A. Vitoria, V. Russo, A. Capelli

Laboratory of Stereoselective Polymerizations (LSP), Department of Chemical Sciences, University of Groningen, 3000 SB Groningen, The Netherlands

Designing catalysts

Collaboration with Moscow State University (MSU), Prof. V. V. Korshak, aims to prepare a series of metallocene catalysts with a combination of Zr, Hf and Ti and to study their activity with different ligands and with various olefins.













































