1ST INTERNATIONAL FibreNet SCIENCE FOR THE PUBLIC DAY

BOOK OF ABSTRACTS

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1st International FibreNet Science for the Public Day

LUCIJA JURKO, MANJA KUREČIČ & RUPERT KARGL

Abstract First international conference in the scope of FibreNet project funded by European Commission. The conference brings the FibreNet together international representatives from industry and academia to discuss opportunities and strengths related to bio-based fibre products. In three consecutive sessions, fifteen international PhD students will present their research results, guide you along the value-chain of fibre-based products and give you the opportunity to discuss the future of bio-based materials.

Keywords: • biobased materials • mechanical properties • paper • packaging • dissemination of research results •

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1st PART

NEW AND ADVANCED PROPERTIES OF BIOCOMPOSITES

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Interfacial Adhesion of Graphene Oxide Adsorbed Flax Yarns with Epoxy Resin

FARZIN JAVANSHOUR, KARTHIK RAM RAMAKRISHNAN, RAMA KANTA LAYEK, PASI KALLIO, AART WILLEM VAN VUURE & ESSI SARLIN

Low density, high specific mechanical properties and favourable environmental profile of natural fibres, such as flax, hemp, kenaf, jute and ramie, make them a potential substitute to traditional composite reinforcements. As in every composite design, strong fibre-matrix adhesion is crucial for efficient stress transfer in natural fibre reinforced plastics. Regardless of hydrophobic chemistry of thermoset resins, they have acceptable bonding with hydrophilic natural fibres compared with thermoplastics. This is mainly due to the high density of reactive functional groups within thermosets such as epoxy. To explore the extent of fibre-matrix adhesion that can be achieved in flax/ epoxy composites, graphene oxide (GO) with various oxygen-containing groups is physically adsorbed on the flax yarns. The microbond results suggest 40 % improvement in the interfacial shear strength of GO treated flax fibres. GO treated flax/epoxy composites demonstrate 14 % and 7 % higher tensile stiffness and strength compared to flax/epoxy composites with 40% volume fraction.

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Compressive Strength of Natural Fiber Composites

VEDAD TOJAGA & SÖREN ÖSTLUND

In many industries (e.g. aerospace, automotive, construction, wind turbine blades etc.), there is a growing interest in the use of natural fiber composites. The main reasons being their good specific mechanical properties and environmental advantages in comparison to conventional composites (e.g. carbon, or glass, fiber composites). In these applications, the primary loads are often compressive. The compressive strength of natural fiber composites is considerably lower than the tensile strength due to fiber microbuckling (e.g. see Fig. 1), which is characterized by strain localization in the matrix material and fiber rotations. The compressive strength is sensitive to fiber misalignments, fiber-matrix interfacial decohesion and the inelastic behavior of the matrix material. It is an important property, but it is difficult to predict. This leads to over-dimensioning of components, higher production costs and ultimately more pollution.

Our recent work [1] presents a model for prediction of the compressive strength. It is based on the rule of mixtures and independent of fiber rotations because it is defined in the reference configuration (i.e. the unloaded state of the composite). It accounts for the microstructure of the composite, including fiber-matrix interfacial decohesion, and enables all types of material behavior of the constituents. In addition, a manuscript that presents a computationally efficient alternative to

plasticity models (e.g. J_2 plasticity) for the inelastic behavior of the matrix material is currently under preparation. The next step under current investigation is an experimental validation of the model. The experiments include compression testing with digital image correlation (DIC) of flax fiber composites containing various matrix materials (e.g. epoxy, MAPP, POM etc.), micro-CT scans and microscopy of the specimens to obtain the fiber orientation distribution, mechanical testing of the composite to obtain an estimate of the fiber-matrix interfacial decohesion and mechanical testing of flax fiber bundles and pure matrix materials to obtain the material behaviour of the constituents. The objective being the development of a convenient and computationally efficient model for design engineers.

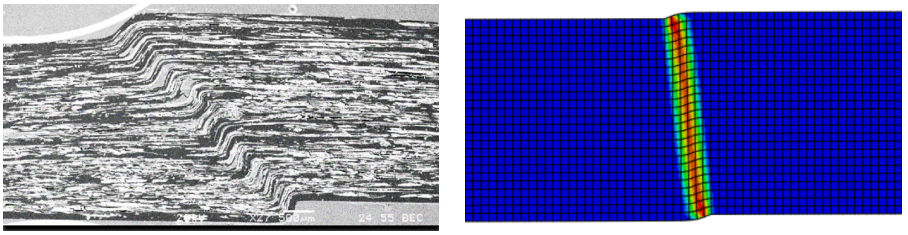

Figure 1: Fiber microbuckling. Experiments by Baley et al. [2] (left) and preliminary simulation (right).

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Accounting of Scope 3 Emission Into a Multiobjective Optimization Model

CARLOS GARCÍA VELÁSQUEZ, SYLVAIN LEDUC & YVONNE VAN DER MEER

The worldwide consumption of plastics has increased in the las few years due to the high requirements for packaging, building and automotive materials. The global economy produced 407 Mt of plastics in 2015, with carbon emissions up to 1.7 Gt of $CO_{2\text{-equivalent}}$ due to the high demand and production of fossil-based plastics [1]. Additionally, the annual plastics production is expected to grow to 1,606 Mt by 2050 [1]. Therefore, we need to find a solution to produce plastics in order to mitigate the environmental impact and economic dependency from fossil resources. In this sense, the use of biomass to produce plastics has arose as a promising alternative solution that can wholly or partly substitute fossil-based plastics. Nevertheless, it is still unclear if the biobased plastics can be produced in an economically viable and environmentally friendly way in comparison with fossil-based materials when direct and indirect emissions are considered in the whole assessment. In this sense, the main goal of this study is to assess the impact of the direct and indirect emissions of the PET production using different feedstock. This work was developed during a summer school in the International Institute of Applied Science Analysis (IIASA) through the Young Scientist Summer Program 2019 (YSSP).

A spatial-explicit optimization model (*BeWhere*) was used to correlate environmental and economic criteria in order to provide a framework that considers the direct and indirect emissions (Scope 3 emissions [2]) to support decision-makers on the design of the value chains. The production of 30%-biobased PET (polyethylene terephthalate) was selected as study case using three feedstock sources: maize, sugar beet and wheat. The techno-economic assessment was used to estimate the production costs of the case study, whereas the Life Cycle Assessment (LCA) methodology was used to estimate the indirect emissions.

The emissions related to the LCA of the PET production account up to 91.4% (wheat case) of the total emissions, whereas the remaining 8.6% accounts to the transportation. The results change depending on the feedstock, the configuration of the supply chain network (transportation network) or the need of fossil PET to supply the current demand.

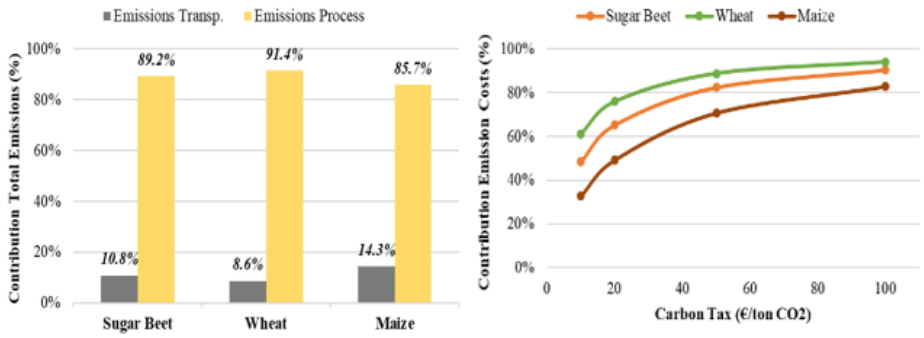

Figure 1: Contribution of the transportation and life cycle assessment emissions throughot the whole supply chain network

Additionally, the economic contribution of the carbon missions in the production costs can account for up to 90% depending on the economic value. Carbon tax is used as a monetization value of these emissions.

As main conclusion, scope 3 emissions should be considered for the environmental assessment of biobased materials, especially when they account more than 85% of the total greenhouse gas emissions. The use of a carbon tax on those emissions is highly important to provide a monetization value that could influence the economic

performance of the process. The integrated use of economic and environmental criteria will help to properly analyse biomass supply chain networks and serves as a powerful decision-making support tool.

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Effect of Transcrystallinity Against Water Absorption in Flax Fibre Reinforced Composite Materials

ALEXANDROS PRAPAVESIS, ESSI SARLIN, PASI KALLIO
& AART WILLEM VAN VUURE

Natural fiber reinforced composites offer interesting properties, such as high specific mechanical and dumbing properties, and coupled with their ecological and renewable nature they have the potential, for specific applications, to outperform traditional materials in the market with minimum impact on the environment. However, one of the main issues that hinder the widespread use of bio-composites is the strong hydrophilic nature of the fibres. Moisture absorption is an unavoidable process that materials have to face through their lifetime, making it a parameter that cannot be ignored during the designing phase of a component. Thereby, in a realistic environment natural fibers have to withstand variable hygroscopic conditions, which lead to water absorption and thus unsteady behavior in their mechanical response due to structural changes in the fiber and matrix cracking due to fiber swelling [1].

It is well recognized in the literature that crystallinity significantly affects the moisture content due to the efficient molecular packing within the unit cell, which creates inaccessible paths to water molecules [3] [4] resulting in more moisture insensitive polymers. When flax is embedded in a polymer melt, the fiber surface may act as a nucleating agent promoting crystallization along the surface. Because of

the high density of the nucleus, the crystallization growth is restricted in the transverse direction forming a crystalline columnar layer, known as transcrystalline layer, across the fibre length [2]. This work studies the potential of the aforementioned crystalline morphology to act as a moisture barrier around the hydrophilic fibers and its influence on the mechanical performance of the bio-composite, before and after water absorption. Polarized optical microscopy was used to observe the crystalline layer between quenched and annealed composites. The results show decrease in the diffusion coefficient and moisture content in equilibrium when transcrystalline layers were present in the composite. The effect of transcrystallinity on the mechanical properties was assessed using 3-point bending test, where it was found improved performance after water absorption, possibly due to the constraining effect of the transcrystalline layer against the fibre swelling.

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2nd PART

NEW AND ADVANCED PROPERTIES IN PAPER AND PACKAGING

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The Effect of Zeta-Potential of Birch Pulp on the Interaction with Dry Strength Agents

MENGXIAO ZHAO, LEIF ROBERTSÉN, TORBJÖRN PETTERSSON, MARI ZABIHIAN, MARKUS KORHONEN & LARS WÅGBERG

Surface charge of fibres plays significant role in papermaking industry, especially the interactions with dry-strength additives. Different levels of zeta-potential of birch fibers has been prepared by removing xylan with enzyme and redepositing birch xylan. Cationic starch, synthetic polyacrylamide (SPAM) and polyelectrolyte complexes (PECs) were investigated as strength additives. Tensile strength, relative bonded areas and scott bond of handmade sheets were characterized to explore the strength properties of papers. In addition, AFM and SEM images were taken to characterize the morphologies of papers. During washing procedures, fines were washed away, therefore tensile strength of both treated pulp decreased. On the other hand, scott bond or z-directional strength of sheets shows different trend.

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Viscoelastic and Viscoplastic Properties of Single Pulp Fibers

MARKO ŽIŽEK & ULRICH HIRN

To understand the properties of paper as a material it is necessary to understand the properties of its building blocks, the single pulp fibers. The two key properties that contribute to the stiffness and the strength of the paper are viscoelasticity and viscoplasticity. In this presentation the viscoplastic and viscoelastic properties of mechanically treated wood fibers are studied by means of dynamic mechanical analysis (DMA).

The fiber samples were glued on the sample holders with 2 component glue and mounted into the DMA. The force-controlled testing protocol consisted of 2 parts. The first part was the recovery testing by exposing the sample to a constant small load for 4 minutes and after that relaxed for 4 min. In the second part the yield point was determined and viscoplastic properties were investigated with cyclic loading, relaxations and recovery until the break. After the DMA testing the cross-sections of the fibers were determined by microtome. The cross-section values were used to calculate the E-modulus, yield stress and breaking stress.

The testing revealed that the fibers are elastic at smaller loads yet when the load is increased they start to show plastic behaviour. The force-displacement curves exhibit a hysteresis at higher loads, that shows the relaxation is time delayed. The DMA testing also proved the yield hardening at loads above the yield point which can be seen in the increase of the slopes. The breaking load is slightly lower than the maximum load in previous cycle. This suggests the presence of cumulative damage in the fibers. Further research is needed to corelate the viscoelastic and viscoplastic behaviour of the fiber with its structure, especially with its fibril angle.

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Evaluating the Degree of Molecular Contact Between Cellulose Fiber Surfaces Using FRET Microscopy

GEORG JOHANN URSTÖGER, MONIKA PATRICIA GASPAR SIMOES,
ROBERT SCHENNACH & ULRICH HIRN

The degree of molecular contact, i.e. the contact area on the nanometer scale, between paper fibers is crucial for the van-der-Waals and hydrogen bond adhesion between the fibers and thus for the fiber-fiber bond strength [1] [2]. We apply Förster resonance energy transfer (FRET) to investigate the degree of contact in the distance range of 1–10 nm between pulp fiber bonds and between thin films [3] [4]. The FRET system with DCCH and FTSC as fluorescence dyes [5] has been validated for spectrophotometry and for local imaging with widefield microscopy, using pHema thin films. Bonding between thin films can be detected with this system, however it has not been possible to achieve a significant FRET signal between bonded pulp fibers (Figure 1). Therefore, we conclude that in principle it is possible to quantify the degree of contact between two surfaces on the nanometer scale with the investigated FRET system. For further work on pulp fibers we recommend an exclusively surface active dyeing, as bulk dyeing massively deteriorates the signal to noise ratio which is likely the reason for the low FRET signal found in this work.

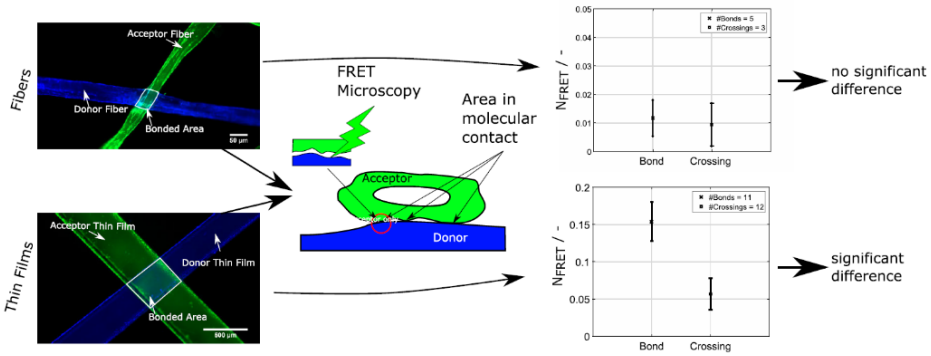

Figure 1:Graphical abstract where we can see both fibres and thin films bonded/crossed and labelled with the fluorescence dyes. In the areas of molecular contact, a FRET signal can be detected.

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The Influence of Anisotropy Variation on the Constitutive Response of Paper Materials: The Insights from Modeling

MOSSAB ALZWEIGHI & ARTEM KULACHENKO

Paper as an engineering material is widely used in various applications from printing to packaging. The usage of paper as a fiber-based material has gradually advanced following the demand for replacing plastics. The production process of paper materials imposes the inhomogeneity and anisotropy properties which make it prone to sudden and stochastic failure that cannot be easily predicted. This problem is shared by some composite materials as well. The main constitutive components of the paper sheet are the fibers which are placed on top of each other stochastically with different orientation during forming and pressing stages. It leads to developing dissimilar properties in different loading directions.

We chose a model-based approach in order to identify the relation between the degree of anisotropy in fiber orientation and the mechanical response of the fiber network. The modeling procedure provides the advantage over the experimental approach through the ability to vary the degree of anisotropy controllably meanwhile imposing the other structural properties such as density, grammage, thickness to be constant at their mean values, which is elusive in the experimental study. In this work, we used a micromechanical model to artificially generate 3-D fiber networks. The fiber network is constituted of fibers, which are deposited on a planar surface

from both sides (up and down) this process is continued until the designated grammage is reached.

The fibers are modeled as a series of non-linear Timoshenko beam elements. Each element has three nodes and quadratic approximation of translational and rotational degrees of freedom. Each node has 6 degrees of freedom (DOF) (3 DOF for translations and 3 DOF for rotation). The beam to beam contact with traction and separation law is used to model bonding between the fibers. A cohesive bond model with linear loading and softening behavior represents the bond failure model. Each one of the numerically generated fiber networks will have a unique degree of anisotropy through controlling the orientation of the fibers during the deposition phase. The anisotropy is computed by measuring the fiber orientation distribution and fit it to an ellipse. The isotropy property is retrieved once the ration between the major and minor ellipse is equal to one.

The aforementioned networks are loaded uniaxially with three different directions namely in MD, CD and with 45°. The stress-strain curves are extracted and used to determine the material parameters for an orthotropic constitutive model based on the continuum approach. In this way, changing the anisotropy will result in presenting different stress-strain response, consequently different constitutive parameters. Based on this, a relation can manifestly be constructed to specify the substantial role of anisotropy on the constitutive response.

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An Introduction to Molecular Dynamics for Modelling Natural fibres

ALI KHODAYARI, AART WILLEM VAN VUURE, ULRICH HIRN
& DAVID SEVENO

Cellulose and its compounds have been the subject of many experimental and theoretical studies for years. However, some features of cellulosic fibres cannot be easily addressed neither through experiments, not through continuum-scale modelling. As an example, there is still debate on reasons behind particular behaviours, e.g. the non-linear tensile stress-strain curve of natural elementary fibres. [1] Additionally, the structure of cellulose crystals has been studied through X-ray scattering or electron diffraction methods but there is not yet enough explanation of the significance of the role of the micro-fibrillar angle on the strength of materials under tensile load. In a more fundamental way, researchers have utilized Molecular Dynamics (MD) simulations to investigate these aspects of natural fibres during the past couple of decades.

An atomistic model of crystalline and non-crystalline cellulose (dislocations) is modelled by MD. [2] The mechanical properties of the models are investigated by performing tensile tests and the difference between the models are characterized based on the torsional angles of different groups of atoms. Results show that a lower mechanical property of the dislocated cellulose can be related to distorted dihedral

angle distributions. These distortions consequently play a role on changing the intra- and inter-chain hydrogen bonding patterns, leading to a shift in stacking of the chains.

The results of MD simulations can be further applied to coarse-grained models, where larger systems can be structured. The intension of these studies is to bridge the findings at the nano-scale to macro-scale.

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3rd PART

NEW BIOBASED FIBRE PRODUCTS IN BIOMEDICAL APPLICATIONS

1ST INTERNATIONAL FIBRENET SCIENCE
FOR THE PUBLIC DAY: BOOK OF ABSTRACTS
L. Jurko, M. Kurečič & R. Kargl (eds.)

University of Maribor Press

Surface Modification of Regenerated Cellulose Fibers Using Carbide Ceramic Particles in Combination with Polyelectrolyte

ÖZKAN YAPAR, ANDREJ ŠTRITOF, FRANCI DEBELAK, RUPERT KARGL,
KARIN STANA KLEINSCHEK & ALENKA OJSTRŠEK

Viscose and other regenerated cellulose fibers have been studied extensively due to their good physical and mechanical properties, softness, excellent processing characteristics and adequate liquid transport properties [1]. Modifying fibers by carbide ceramic particles (SiC and ZrC) is one approach to impart special functionalities, e.g. temperature resistance or thermal conductivity. In order to enlarge the binding efficiency and washing durability of these particles on the fibers surfaces, some extra binding/crosslinking compound should be added before or during the particles' application.

The aim of presented work was firstly to embed carbide ceramic particles on the viscose fibers and secondly, to evaluate newly obtained properties. Thus, fibers surfaces were pre-treated with a selected cationic polyelectrolyte and further coated with sodium carboxymethyl cellulose in water containing $CaCl_2$ together with ceramic particles. Finally, washing and drying procedures were accomplished and samples were stored in a desiccator for further characterization. The influence of

pre-treatment and different exhaustion parameters, i.e. concentration of CMC and ZrC, temperature were studied with the aim to obtained optimal conditions for sufficient and durable coatings. Functionalized surfaces were analyzed using Scanning Electron Microscopy (SEM). Tensile properties of the fibers were determined by a Vibrodyn 500 from Lenzing Austria. Fiber surfaces charges were analyzed by potentiometric titrations and optical properties by spectrophotometric measurements.

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Cellulose Aerogel Fibres: Development of a Multi-Functional Wound Dressing

MATIN ROSTAMITABAR, GUNNAR SEIDE, STEFAN JOCKENHÖVEL & SAMANEH GHAZANFARI

Introduction

Porous cellulose aerogel fibres with high porosity, low density and high specific surface area can be a suitable candidate to design multi-functional wound dressings. The structure of the nano-porous network inside the fibres can be tuned based on the release profile of each bio-active agent that covers a particular phase of the wound healing process.

Materials and Methods

Cellulose is dissolved in molten salt hydrate of $ZnCl_2$. The high viscous solution of the cellulose (5-6% w/w) is spun by a customized wet spinning line at 70 ^oC and regenerated in ethanol or isopropanol. The obtained salt free alcogel fibres (ϕ=100-500 μm), could be impregnated by supercritical CO_2 methods such as solvent exchange or post treatment. In solvent exchange, the alcogel fibres could be immersed in a drug solution then introduced to the autoclave for in-situ drying and impregnation. However, in post treatment process, first pure aerogel fibre is dried

with SCO_2 then it is placed in the autoclave again for impregnation. In this study, four different model drugs including Vitamin C, Methyl blue, Fluorescein and Rhodamine B were investigated.

Results

The white opaque aerogel fibres were obtained after SCO_2 drying with a shrinkage of 15 ± 5%. The mechanical properties of the fibres showed to be dependent on the cellulose concentration, the type of solvent and the fibres diameter. Fibres strength is rather low, for example 1 N is the max. tensile force for sample with dimeter of 200 μm. Scanning electron micrographs (SEM) of the aerogel fibres cross section shows a porous mesh of randomly oriented cellulose nano-fibrils connected in 3D with pore sizes ranging from 10-200 nm (Fig.1). The drug release measured in PBS (pH 7.4 and 37 °C) proved to be diameter depended and a high amount of drugs is released in less than 200 mins. X-ray microtomography showed that the fibre structure consists of 63% open porous and 0.01% closed Porous (Fig.2). In addition, using XTT assay the viability and proliferation of fibroblast cells in contact with cellulose fibres was measured. In some samples, small traces of trapped salt reduce the proliferation rate, requiring further washing of alcogel fibres after regeneration.

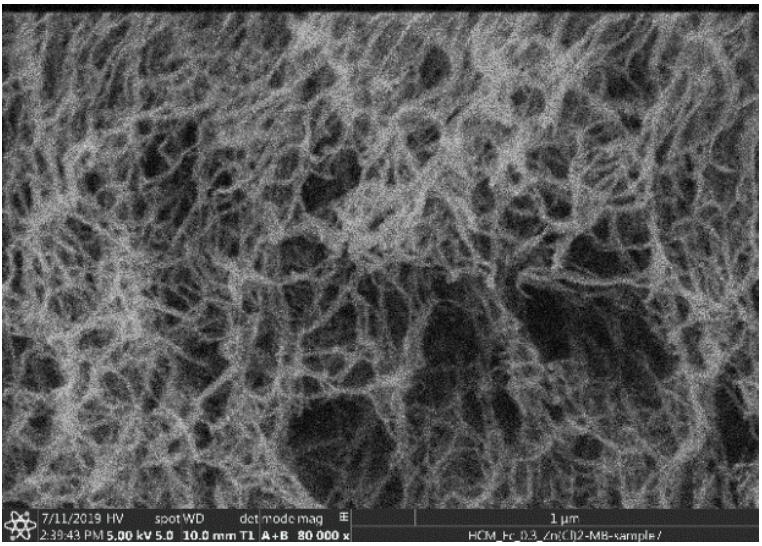

Figure 1: Scanning electron micrographs of cellulose aerogel fibers obtained by isopropanol regeneration and supercritical CO2drying (6 wt.% cellulose content).

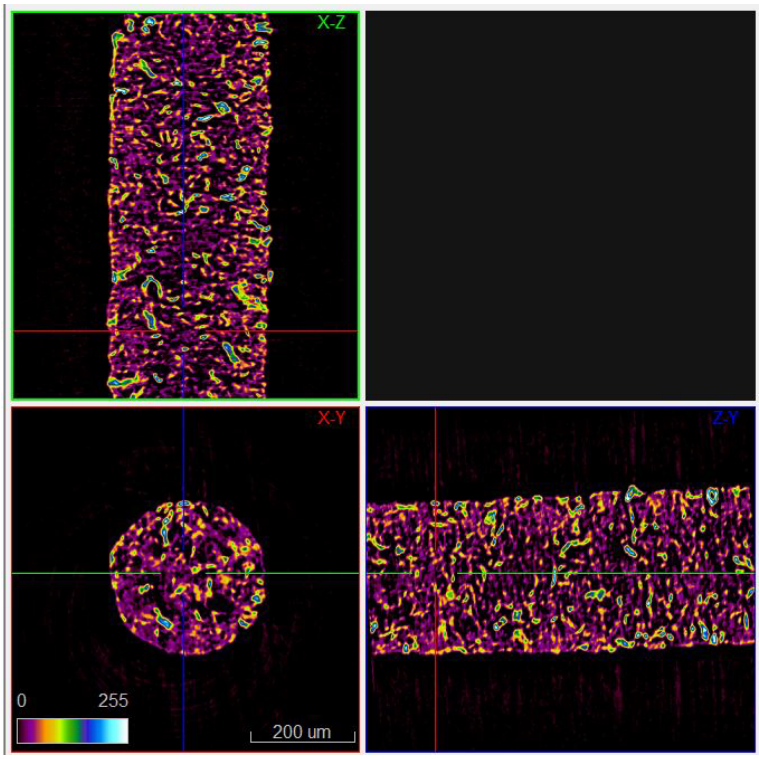

Figure 2: X-ray microtomography (Micro CT) of cellulose aerogel fibers, reconstruction-using CGLS with 10 iterations, resolution 0.8 micrometer

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Antimicrobial Electrospun Carboxymethyl Cellulose and Polyethylene Oxide Based Wound Dressings

LUCIJA JURKO, MARTIN SIMON THONHOFER, SILVO HRIBERNIK, CHRISTIAN SCHMITZ, LUKAS FÖRSTER, TAMILSELVAN MOHAN, MANJA KUREČIČ, KARIN STANA KLEINSCHEK & RUPERT KARGL

Chemical derivatization of polymers is a common approach to increase biocompatibility, decrease toxicity or add various chemical functionalities. [1] [2]. The aim of this work is to introduce a pH-independent positive charge into polyallyamine hydrochloride (PAH) by an amide bond with betaine hydrochloride. Electrospun fibers should be formed with this derivative in combination with carboxymethyl cellulose (CMC) and polyethylene oxide (PEO). Resulting materials could be used as antimicrobial wound dressings. 1-Ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) in combination with N-Hydroxysuccinimide (NHS) have long been proven as efficient coupling agents to form amide bonds. This chemistry was investigated here for betaine hydrochloride and PAH.

Characterization of the product was conducted by attenuated total reflectance Fourier transform infrared spectroscopy (ATR-IR), ^{1}H, and ^{13}C NMR spectroscopy. Based on the obtained results it can be concluded that a novel cationic PAH derivative has been synthesized. As confirmed by scanning electron microscopy, the cationic product is spinnable into nanofiber webs when combined with CMC and

PEO. The concentration of the cationic product was calculated in accordance to minimum inhibition concentration towards *E. coli* and CMC as a biogenic biocompatible fibrous polymer. Determination of the minimum inhibition concentration (MIC) of quaternized polyallylamine against *E. coli* showed a good antimicrobial activity. Further investigations target more detailed antimicrobial testing and biocompatibility studies of the quaternized polyallylamine and possible application of the nano-fiber webs as wound healing materials.

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University of Maribor Press

Automation in Fiber Characterization

ALI ZAREI & PASI KALLIO

Cellulose fibers are very strong with impressive ability in bonding; considering the objective of end-product paper properties, the understanding of suitable properties of fibers, is a challenging topic for research and developments in pulp and paper industry [1]. The mechanical characterization of paper fibers and paper fiber bonds directly implies the mechanical properties of paper.

One of the most important parts in tailoring bio-based fibers is characterization of mechanical properties. Currently, a vast amount of time of our scientists is being wasted on manual sample manipulation [2], test monitoring, data trimming, statistical analysis and so on. By using machine vision and machine learning algorithms, we are trying to automate tests on mechanical properties of fibers (Fig.1). This intelligent platform is aimed to be based on deep learning techniques such as Convolutional Neural Network (CNN), Recurrent Neural Network (RNN) and in further scope using Reinforcement Learning. Another part of our objectives is to enable our system to detect failures during manipulation and measurement process; subsequently it would be capable of adaptive decision-making for boosting up the characterization and skipping the manual time consuming parts.

Finally, the desired platform is a modular and scalable software package which enables our micro-robotics platform to manipulate samples with an automatic process surveillance at microscale.

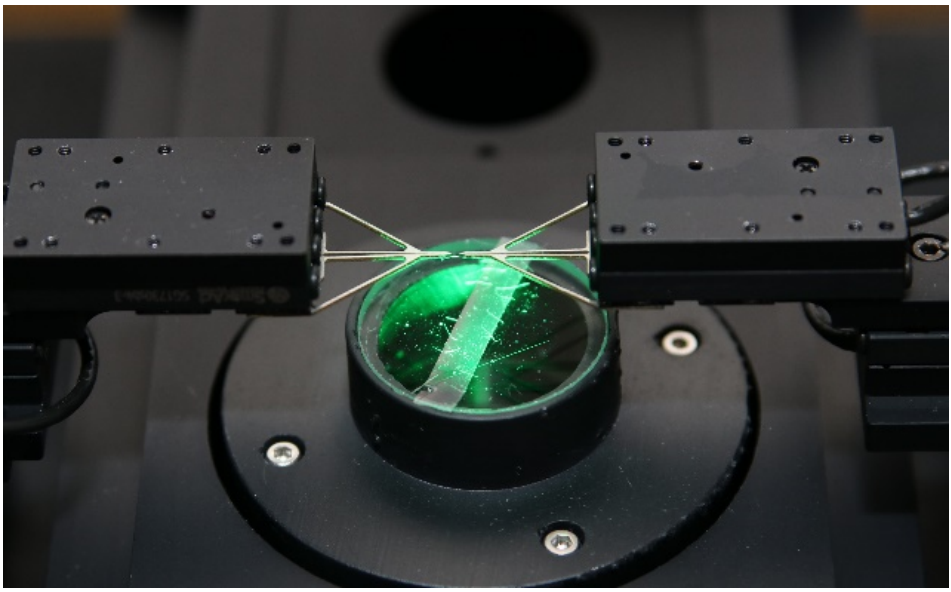

Figure 1: Micro-robotics platform; tensile testing of paper fibers

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Synthesis of Polysaccharide Derivatives for Cardiovascular Tissue Engineering Applications

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KARIN STANA KLEINSCHEK & TAMILSELVAN MOHAN

Cardiovascular diseases are disorders of heart and blood vessels and the leading cause of death in the world. Traditional treatment is the transplantation of autologous healthy blood vessel via bypassing diseased vessels. Alternatively, artificial vascular grafts have gained a great interest. [1] For example, polyester-based grafts with inner larger-diameter (> 6mm) are readily available for the clinical use. However, they are not suitable for small-diameter vascular graft applications since thrombosis and occlusion can still occur on the luminal surface of the graft. [2] Many approaches including surface modification, optimization of mechanical and structural properties have been introduced to enhance the biocompatibility and growth of endothelial cells (ECs). [3] 3D printing is an advanced method currently used in vascular tissue engineering application because of its feasibility to create patient-specific grafts and control over fabrication. [4] [5] For such application, choosing appropriate biomaterials as a ink is a key parameter for the proper design of the grafts. These biomaterials must be degradable, cost effective and sustain its structure for time period enough for allowing complete endotheilization. [6] This work aims to prepare amino-acids modified polysaccharides (PS) and use them for creating vascular graft by 3D printing technique. These modified PS brings new functionality, optical

properties, and can be used to increase of hemocompatibility, mimic the components of extracellular matrix of vascular tissue, improve the ECs adhesion, and to prevent the unspecific protein adsorption.

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