MSc in Chemistry and Materials engineering
Master Thesis subjects 2022-2023
proposed by

Physical Chemistry and Polymer Science (FYSC) / Department of Materials Science and Chemistry (MACH)

1. Sustainable self-healing polymers for soft robotics

Summary:
Soft robotics is a field focused on studying the use of flexible and compliant materials as components for building robots instead of rigid traditional materials, such as metals. The field of soft robotics is moving really fast in the last years as soft robots are developed with new capacities, materials and designs. In collaboration with the Robotics and multibody mechanics (R&MM) research group, we have developed self-healing robots capable or recovering from damages such as punctures or scratches. These self-healing materials are based on the reversible Diels-alder reaction between a furan and a maleimide functional group. Using this chemistry, we can synthesize materials that can heal severe damages with an efficiency close to 100%. Nevertheless, there is still work to do to bring these materials to commercial applications. In this sense, one of the most urgent matters faced is the improvement of their sustainability and avoiding the usage of dangerous chemicals. The main objective of this thesis will be to explore new bio-based and sustainable raw materials, such as the ones shown in Figure 1B, to substitute the current materials used for the self-healing polymers. Promising results have been already obtained using oil extracted from castor seeds. The student will contribute to the optimization and development of this material. Nevertheless, motivated students are encouraged to propose their own approaches, the viability of which will be evaluated before the starting of the thesis.

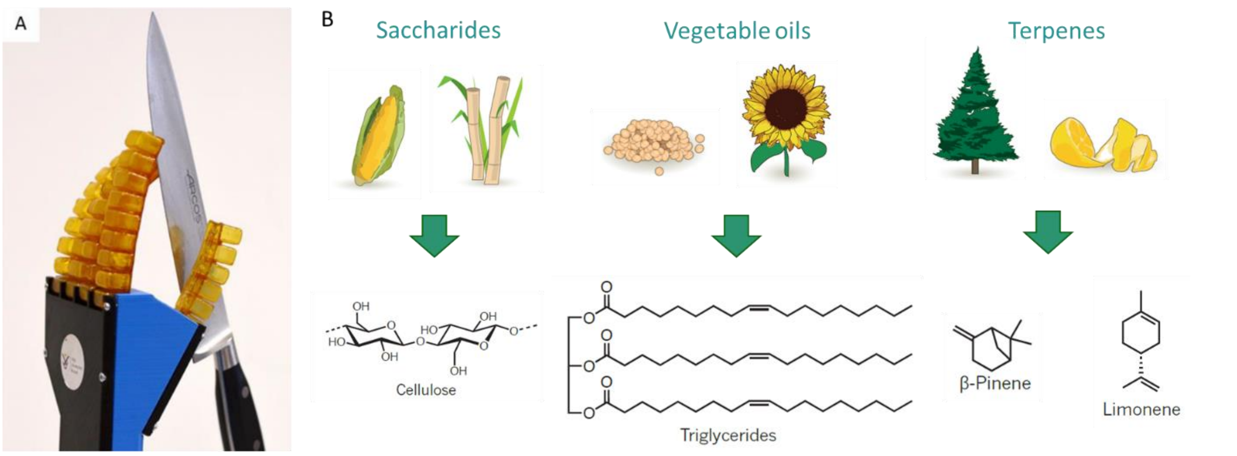

Figure 1 A) Self-healing soft pneumatic hand demonstrator build using Diels-Alder polymers. B) Some examples of bio-based sources that can be used in the synthesis of polymers.

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2. Self-healing foams for soft robotic applications

Summary:

Reversible covalent polymer networks offer a number of advantages compared to permanently crosslinked polymer networks. The reversible nature of their crosslinking chemistries enables **reprocessing and recycling** of polymer networks in foams, rubbers, thermosets and composites. Moreover, these materials possess the ability to heal damage. This **self-healing** ability results in the recovery of their initial properties and performance, thus extending the service lifetime of the materials and products.

In this work, the self-healing properties and recyclability will be assessed in more complex material morphologies. The initial focus will be closed-cell foams and can be extended to other hollow structures (e.g., metamaterials) or phase separated blended material morphologies. Foams find many applications in soft robotics, exploiting among others their light weight, impact, shock absorption and auxetic properties.

This work is performed in collaboration with the Brubotics group of Mechanical Engineering at VUB.

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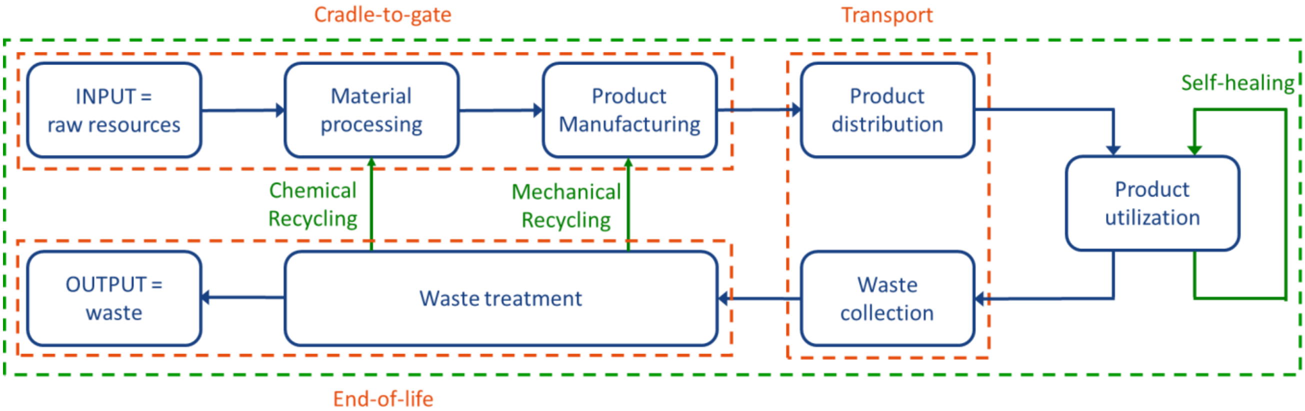
3. Lifecycle assessment framework for self-healing materials and products

Summary:

Reversible covalent polymer networks offer a number of advantages compared to permanently crosslinked polymer networks. The reversible nature of their crosslinking chemistries allows **reprocessing and recycling**. These are major improvements compared to their irreversible counterparts that find widespread use in construction, transport, sports and other industries. Reversible polymer networks have the possibility to replace poorly recyclable polymer networks in foams, rubbers, thermosets and composites, provided that they can offer the same excellent mechanical properties and the necessary thermal and chemical stability, combined with improved reprocessability. Moreover, these materials possess the ability to heal damage. This **self-healing** ability results in the recovery of their initial properties and performance, thus extending the service lifetime of the materials and products.



No framework exists to date that accounts for the service lifetime extension via self-healing in the sustainability assessment of this new class of self-healing materials. Often lifecycle assessments limit to cradle-to-gate or even gate-to-gate evaluations and comparisons. During this thesis work, a method will be developed to assess the impact of self-healing on the lifecycle of self-healing materials and products. In addition, the sustainability improvement offered by reversible covalent polymer networks will be assessed with comparison to current chemical and mechanical recycling methods available for rubbers, thermosets and related composites. This work will be performed in collaboration with Intelligence in Processes, Advanced Catalysts & Solvents of Universiteit Antwerpen.

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4. Design of a low-cost prosthetic liner for developing countries

Summary:

An estimated 40 million people living in developing countries need a prosthetic. Millions of these amputees live in central Africa, while only about 5-15% of these patients receive a prosthetic limb. Ugani Prosthetics is a social entrepreneurship that wants to tackle this scalability issue. 3D printers and 3D models have been around for many years, but they don't seem to get to the people who need them the most. Ugani Prosthetics' goal is

to create impact on a large scale, by quickly expanding local manufacturing capabilities, and expanding to different cities and countries with a proven business model.
As you can see from the images below, we already have a design for a socket that is slightly adaptable to change together with the leg throughout the day. Inside of this socket, the patient needs to wear a liner, which is a sort of sock that fits around the stump. Today, liners are made out of silicone, thermoplastic elastomers, urethane or other soft materials. They drastically increase the comfort of the patients as they reduce friction and wounds on the stump. They can cost several hundreds of euros, meaning that they double the cost of our prosthetics.
As the liner is a vital part of every prosthetic, the goal of this master thesis is to improve the existing designs. New materials and production techniques have to be researched, just as new and better designs. Alternatives like cushions in the socket are also a possibility. The liner should be low cost, comfortable, easy to produce and durable. Additionally, it should reduce sweating as our patients live in a hot and humid climate and transpiration can cause irritation of the skin.



This project is in collaboration with a mechanical engineering master thesis student at the Robotics & Multibody Mechanics research group of the Mechanical Engineering department and with Ugani Prosthetics.

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5. Thermomechanical properties and crystallization behaviour of PHA biopolymers

Summary:

Polyhydroxyalkanoates (PHAs) are microbiologically produced, biodegradable and biocompatible polymers which have been attracting considerable attention as a sustainable alternative for petroleum-based thermoplastic polymers. However, fundamental knowledge on the structure-property relations of PHAs is still lacking, especially for less common copolymers such as poly(3-hydroxybutyrate-co-4-hydroxybutyrate), which is a very promising material for high value-added applications as biomaterial in the biomedical industry. Therefore, the goal of this project is to study the thermomechanical properties of microbially synthesized P(3HB-co-4HB) samples with varying structural properties by, among other techniques, differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). Because poor processibility due low crystallization rate of P(3HB-co-4HB) is known to be one of the major drawbacks of this material, the crystallization kinetics of these biopolymers will also be studied. In addition, the possibility of enhancing the crystallization rate by addition of biocompatible nucleating agents will be explored. This is a broad topic, meaning that it may be possible to accommodate two students, specializing in different aspects.

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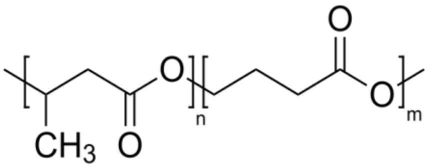 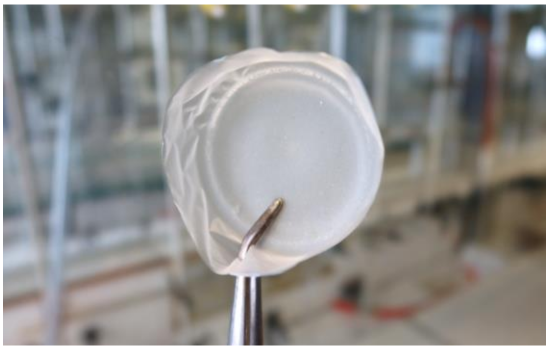

Chemical structure and solvent cast sample of biosynthesized P(3HB-co-4HB)

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6. 3D printing concrete with copper slag-based hybrid cement

Summary:

Copper is a well-known metal used extensively in engineering applications. However, the residue produced during copper extraction from its ore remains a problematic waste currently stored in large ponds, or dried and stored in heaps. Over the recent years, this non-ferrous metallurgical slag has gained extensive research interest as a major precursor of inorganic polymers and cementitious blends. However, its application in the novel hybrid cement remains very limited. Thus, this study aims at developing an alternative binder, which contains a large proportion of copper slag > 70 wt%, a small proportion of Ordinary Portland Cement < 30 wt% (OPC), and an alkali activator, so that it can be used in 3D printing concrete (3DPC) as the binder. In this work, on the one hand, the setting time, the rheology properties (i.e., plastic viscosity, yield stress, etc.,) and hydration behavior for this hybrid cement will be evaluated and compared to other binders that have been successful in 3DPC to ensure its printability. On the other hand, the carbon emission and economic costs will be calculated and compared with the successful binder in 3DPC from an environment-friendly/low-carbon view.

Keywords: 3DPC; hybrid cement; copper slag; low-carbon.

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7. Research on stone wool growing media

Summary:

Grodan, part of the ROCKWOOL group, develops and produces stone wool growing media for the horticultural sector. These innovative materials are used for the cultivation of vegetables and flowers, such as tomatoes, medicinal cannabis, roses, etc. By applying precision growing principles these products lead to higher crop yields with significantly less use of energy and natural resources, like water. Stone wool growing media consist of stone wool fibers held together by a thermoset resin binder, which makes highly porous materials that are typically hydrophobic in nature. For Grodan, on the other hand, the material has to be hydrophilic as plants need water (and nutrients) to grow and produce flowers or vegetables. For this purpose an additive is added during the stone wool production process. The efficiency of this additive and the resulting water characteristics of the stone wool substrate strongly depend on the compatibility with the selected binder system, the resulting morphology and the applied cure conditions during production. It would be of interest to examine the stability of the water characteristics of the stone wool substrate and whether these change by external factors. The influence of the wetting agent-binder combination on the stone wool properties requires continuous investigation, especially since binders keep on evolving to make Grodan products more sustainable. Additionally, alternative end of use routes are being explored for improved sustainability, which also needs further research.

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8. Frontal Polymerization

Summary:
Frontal polymerization is a method of rapidly converting monomer to polymer through the propagation of a localized reaction wave. It is an energy-efficient way to produce high-T_g thermosets, but also finds applications for elastomers and hydrogels. In frontal polymerization, a small energy input in one point initiates the reaction, which through its exothermicity and its acceleration with increasing temperature leads to the generation of a reaction wave, rapidly progressing through an entire mould or coating and turning the liquid monomer into a rigid polymer. In this project, we want to study the effect of heat losses on the stability of polymerization fronts. This will involve both experimental work (designing test setup, studying polymerization kinetics) and heat transfer and reaction modelling.

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9. Preparation and characterisation of textile reinforced alkali-activated thin composites

Summary:
Traditional steel reinforced constructions can resist higher impact and load than non-reinforced. Yet to protect from corrosion, thick panels or blocks are necessary, increasing costs and environmental impact (i.e. in production and construction). Technical textiles can circumvent the issue of corrosion and could even reinforce thin panels, avoiding the necessity of thick ones. To reduce the environmental impact even more, alkali-activated materials could substitute conventional cement. In this project, industrial residues such as copper slag or bauxite residue will be preferably used for the development of the alkali-activated matrix, in order to contribute in their recyclability, sustainability and circular economy. The work on optimization of matrix workability, suitable textile selection, optimal fibre volume fraction, textile - matrix interactions and thermal stability of the prepared composites will be considered in the project. Analytical techniques such as X-ray fluorescence, X-ray diffraction and TG/DSC will be used to characterise the precursor for matrix development, meanwhile calorimetry, impulse excitation technique, Resonalyser, elastic modulus record on heating and flexural strength will be used to characterise the prepared matrix and composites.

Key words: Alkali-activated material, textile reinforced thin composites, recyclability, sustainability, thermal stability, construction application.

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10. Ecological cements from metallurgical residues via temperature and/or hydrothermal route (< 60 °C)

Metallurgical slags have a great potential for being recovered and valorised as “green” building materials.

Belonging to the family of alternative cementitious materials, inorganic polymers (IP) are rising in importance because of the drive to decrease CO_2 emissions of concrete production, while delivering comparable or even superior properties, i.e., compressive strengths reaching up to 80 MPa.

Research in inorganic polymers (IPs) is expanding to ferrosilicate precursors, such as slags from the non-ferrous metal industries. Although IP binders have been studied for several decades, question marks about their reactivity, effect of some elements on the reaction kinetics and mechanism, as well as on binder structure and properties remain unclear.

The scope of the current research thesis is to develop and evaluate different approaches to produce a load-bearing porous building block (LPBB) for construction use. Properties, of the developed LPBB shall be comparable to those of existing commercial products, while having a considerably lower environmental impact and therefore an advantage in the competition.

In more detail, this work focus will be on using a reactive slag to be combined with the high-alkaline activating solutions that will generate a lightweight porous material with desire properties at room or slightly elevated temperatures (i.e. up to 60oC). The lack of post-processing will provide a major advantage concerning the environmental impact of the final product. A moderately elevated curing temperature could promote compressive strength development and lead to a homogeneous geopolymer structure.

The mix designs will be tailored by means of additives in order to achieve rheological behavior and setting time suitable for making porous products. The produced foams will be eventually cured slightly elevated temperatures and evaluated with respect to their mechanical and physical properties.

This work is part of an Vlaio project, with the participation of Wienerberger and Metallo Group.

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11. Ecological cements from metallurgical residues via sintering (300 °C – 900 °C)

Metallurgical slags have a great potential for being recovered and valorised as “green” building materials.

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In more detail, the focus of this work is to develop a porous product of minor mechanical properties at room temperature that will transform into a glass-ceramic based porous material after firing. The focus will be on compensating the environmental impact associated with the firing by drastically reducing the amount of alkalis (used as activator) as well as using coarser (less milled) input materials.

The mix designs will be tailored by means of additives in order to achieve rheological behavior and setting time suitable for making porous products. The produced foams will be eventually cured slightly elevated temperatures and evaluated with respect to their mechanical and physical properties.

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12. **Nanocellulose reinforced cementitious composites**

Summary:

Nanocellulose is a nanomaterial with a nanometer scale in its diameter and consists of many hydroxyl groups on its surface. These hydroxyl groups, which can be used for surface modification, with strong hydrogen bonding networks give excellent physical and chemical properties to fiber cellulose and makes it strong. Low weight, low density, and strength are some properties of nanocellulose. Nanocellulose extracted from plants can be achieved from trees, shrubs, different herbs, grasses, flowers, and so on. Some other significant plant sources are sugar canes, grass, bamboo, rice husk, corn and pineapple leaf, carrot, sisal, etc. The fascinating properties of nanocelluloses such as high surface area, considerably improved mechanical and optical properties, low density, low cost, biodegradability, great strength, and stiffness bring remarkable impacts on the properties of cementitious materials. Cellulose nanocrystalline (CNC) can be extracted by different types of treatment methods such as mechanical, chemical, and enzymatic. In this project, the first step is the extraction of CNC from different biomass resources by acid hydrolysis, and the next is using these CNCs in producing cementitious composites. In addition, the volume fraction of CNC, dispersion of CNC in the matrix, degree of hydration, workability, shrinkage, durability, microstructure, and mechanical properties should be investigated.

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