Contract No:

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Title of Project Functionalized Cellular Magmatics

Project Start and End Dates Project Start Date: 10-1-2020

Project End Date: 9-30-2022

Project Highlight

Engineered cellular magmatics, a disruptive transformation of foam glass technology, convert the enormous amount of wasted glass stored in landfills into advanced, valorized materials with applications ranging from geotechnical fill to environmental cleanup. SRNL is capitalizing on decades of glass and ceramics science research to pioneer the fundamental concepts that will establish engineered cellular magmatics as a material of the future: economically advantageous and environmentally conscious.



Project Team

Principal Investigator: Cory L. Trivelpiece, PhD Team Members: Robin L. Brigmon, PhD Madison Hsieh Alex Kugler, PhD Austin Stanfield, PhD

External Collaborators (all external collaborators and their respective organizations that participated in this project: Collin Wilkinson, PhD, GlassWRX LLC Robert Hust, GlassWRX LLC

Abstract

We are pioneering the development of fundamental and applied research related to engineered cellular magmatics (ECM) technology. Over the course of our first year, we developed the methodology and measured the effects of various additives on ECM properties. We demonstrated the ability to control the phase and morphology of post-process secondary minerals on ECMs based on starting conditions and compositions. Both achievements are critical to advancing the use of ECMs for applications such as water filtration and runoff remediation. We established the ability to grow various microbiologic consortia on ECM surfaces as well as a process that allows industrial scaling of the technology for rapid field deployment in applications such as the cleanup of fossil fuel contamination. Furthermore, this biotechnology also has potential application in the nascent fields of biomining of precious metals and bioremediation of toxic heavy metals.

Objectives (Year 1)

- Establish lab-scale ECM synthesis
- HTXRD of synthesis reactions
- DSC/TGA of synthesis reactions
- Substrate/lattice testing of commercial products

Date
Date
Date

4. Intellectual Property Review:

This report has been reviewed by SRNL Legal Counsel for intellectual property considerations and is approved to be publicly published in its current form.

SRNL Legal Signature

Name and Signature

Introduction

The U.S. is the largest generator of waste per capita in the world and currently ranked 25th in Global Waste Index scoring out of 36 countries in the Organization for Economic Cooperation and Development in terms of overall waste management¹. Many factors play into this ranking, chief among them the fact that the United States is one of the least densely populated developed nations – in other words, we have the space required to landfill large amounts of municipal solid waste (MSW). By landfilling this material, we are also discarding untold billions in wasted resources. An Accenture analysis estimated that \$1T dollars of untapped resources are sequestered in landfills across the globe annually².

One of the most technologically unwarranted of the squandered resources is post-consumer waste glass. Glass is sometimes colloquially referred to as an "infinitely recyclable" material, and the technical implication is that glass can be recycled numerous times without drastically altering the properties for which the original composition was fabricated. Unfortunately, glass recycling is not economically viable within the current national waste management strategy, which means that a large majority of glass that gets disposed in the United States – *even glass that has been recycled "curbside" – ends its lifecycle in a landfill.* Some estimates put the amount of glass entering the recycling stream only to be landfilled after sorting at a recycling facility as high as 85%. This waste of a manufactured resource presents a unique opportunity for SRNL: capitalize on our decades of experience as world leaders in nuclear waste glass and ceramic science to transition into a new research area of focused, fundamental science coupled with the circular economy and emergent industrial philosophies to develop sustainable solutions that will enhance the laboratory's leadership in glass and ceramic science while solving real-world problems that impact the national environment and economy.

The proposed research serves many goals: 1) to understand the fundamental reactions occurring during ECM synthesis in the presence of additives to the base formula. 2) To investigate the efficacy of commercially available ECMs as biological substrates for microbiologies known to have hydrocarbon/contaminant remediation capabilities. 3) Establish ECM science as a new, niche research area at SRNL.

Approach

This project is guided by an overarching principle that seeks to understand the fundamental aspects of ECM synthesis, for example the underlying phenomena that control interfacial reactions between additive and glass surfaces during processing, while guiding experimental progression towards the pragmatic application of these fundamental discoveries (Figure 1). We focus strongly on the practical applications of our work as part of the project is to integrate nascent breakthroughs as quickly as possible into commercialization of products within a circular economic model. At the same time, we are establishing a foundation of underlying, elemental science from which many new research directions can be pursued.

To date, the work has been conducted in two parallel paths: The first path is focused on the aforementioned fundamental synthesis science. The experiments are centered on understanding reaction mechanisms, mineralogical speciation, chemical and mechanical properties, etc. We employ techniques such as high-temperature X-ray diffraction, differential scanning calorimetry, and thermogravimetric analysis to investigate these phenomena. In addition, we also utilize physics-driven machine learning and cutting-edge glass theoretical science (e.g., TCT, toy landscapes) to model these phenomena allowing us to make theory-based predictions about process/product optimization as well as reduce the number of

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experiments required to understand elemental aspects of the research. The second path, arguably more applied yet still fundamental, involves the coupling of ECM physical science with biotechnology. We are studying how microbiological films interact with ECM surfaces utilizing specific biological consortia that have demonstrated efficacy at the remediation of environmental contaminants. In addition, we are developing approaches that enable the industrial-scale production of ECM/biofilm materials for economical, large scale deployment. We employ techniques such as flow cytometry, scanning electron microscopy and optical methods to understand how ECM properties like composition and porosity affect the development of biofilms.

Accomplishments

- Measured the thermal phenomena governing the reactions between 15 different additives mixed with recycled glass cullet observing effects such as changing of the cullet liquidus behavior by as much as 100 °C. (Figure 2)
- Determined experimentally and confirmed through simulations that secondary mineral phase growth is significantly more linked to environmental thermodynamics as compared to ECM composition provided the necessary phase ingredients are present. (Figure 3)
- Proved the viability of using commercially available (i.e., non-optimized) ECMs as substrates for biofilms including the growth of various microbes with known remediation capacities. (Figure 4)
- Demonstrated a technique for preserving the ECM/biofilm structure that enables the storage and deployment of the materials at industrial scales. (Figure 5)

Future Directions

- Continue fundamental investigations of the controlling phenomena at the glass/additive interface. This includes determinations of combinatory effects of additives, which will rely on experimental and computational solutions to develop a cohesive strategy for process/product optimization
- Determine the efficacy of ECMs with specific mineral phases (primary and secondary) at the remediation of environmental contaminants. We will measure this effectiveness at the laboratory scale during the next phase of the work.
- Quantify the effects of secondary mineral growth on the physical properties of the ECM. We will determine how properties such as the ECM's load bearing ability are affected by the evolution of secondary mineral phases during post-processing techniques.
- Quantify biofilm growth rate based on ECM composition and physical properties. These experiments will determine how characteristics like mineralogy, porosity, and pore size affect the growth of biological consortia.
- Measure the efficacy of ECM/biofilm combinations at hydrocarbon removal from various media such as soils and solutions. Additional experiments will explore the potential for remediation of other types of contamination like heavy metals from similar media.
- Continue to explore external funding opportunities in areas that have been informed by the initial work as they relate to ECM technology. (Figure 6)

FY 2021 Peer-reviewed/Non-peer reviewed Publications

• Wilkinson, C, Trivelpiece, C, et al. Hybrid Machine Learning/Physics Predictions of Oxide Glass Formability, Acta Materialia, accepted. (I.F. 8.2)

Intellectual Property

• N/A

Total Number of Post-Doctoral Researchers

- Alex Kugler, PhD SRNL postdoctoral researcher (on-site)
- Austin Stanfield, PhD SRNL postdoctoral researcher (on-site)

Total Number of Student Researchers

• N/A



Figure 1: The research conducted under this LDRD seeks to understand the fundamental aspects of ECM synthesis as they relate to optimizing material designs for pragmatic solutions such as the remediation of environmental contamination caused by industries such as fossil fuel extraction and agriculture.



Figure 2: The thermal effects of 15 additives have been measured for their individual impact on the behavior of the glass/additive system during processing via differential scanning calorimetry. Some additives can alter glass properties like transition temperature by as much as 100 °C while others affect the crystalline phases that form during synthesis.



Figure 3: The temperature dependence of the growth of secondary mineral phases was confirmed experimentally (A) as well as with modeling (B). At $T_{growth} = 90$ °C, the rate of growth is exponentially faster than at 50 °C. The primary mineral phase identified in the 90 °C sample was zeolite NaP, which has a well-known capacity for cation exchange.



Figure 4: Biofilms were grown on commercial ECM substrates at lab-scale, and a method for preserving these biofilms for field deployment was developed. This growth and preservation method is economically scalable for industrial processes and large-area deployment.



Figure 5: The ability to reactivate preserved films was confirmed for various initial incubations times. We observed that the lack of difference between 72 h and 196 h of incubation drastically reduces the economy of scale for this technology.



Figure 6: This current research and other products have informed several areas of research and we anticipate that many more will be generated as a result of further discoveries through this LDRD.

References

1. . Available from: <u>https://sensoneo.com/sensoneo-global-waste-index-2019/</u>.

2. Lacy P, Rutqvist J. Waste to Wealth - The Circular Economy Advantage. New York, NY: Palgrave Macmillan; 2015.