MATERIAL HISTORIES: The Future of Materials Design

Gannon Murray[1], David Elbert[2], Brandon Wilfong[3], Tyrel McQueen[3]
[1]Department of Chemistry, Earlham College, Richmond, IN, 47374
[2]Hopkins Extreme Materials Institute, Johns Hopkins University, Baltimore, MD, 21218
[3]Department of Chemistry, Johns Hopkins University, Baltimore, MD, 21218

https://occamy.chemistry.jhu.edu

https://www.paradim.org/

Introduction

As the demands of materials research and design shift towards data-driven approaches, it is important that laboratories develop data collection procedures to ensure they do not fall behind. In addition, the Materials Genome Initiative (2011) and Nelson Memorandum (2022) promote the prompt adoption of public data sharing by federally funded research. In the wake of these trends, a need arises for metadata instantiation methods that are both robust and accessible.

This study serves as a proof-of-concept for the end-to-end implementation of the Graphical Expression of Materials Data model. This model allows for the development of Material Histories which contain experimental metadata for an experimental procedure. In this project instantiation procedures were developed and utilized to capture syntheses of Yttrium Orthovanadate (YVO_4). YVO_4 is a crystal with a tetragonal zircon structure and has applications in optics and quantum transduction.

Graphical Expression of Materials Data (GEMD)

GEMD is an open-source schema developed by Citrine Informatics for storing interconnected data objects, or nodes. GEMD node types include materials, processes, measurements, and ingredients as depicted in Figure 1 below. Nodes can have associated property, condition, and parameter attributes as well as any number of tags and unique identifiers (UUIDs).

This data model allows for the intuitive instantiation of experimental metadata in a flexible, machine-readable format.

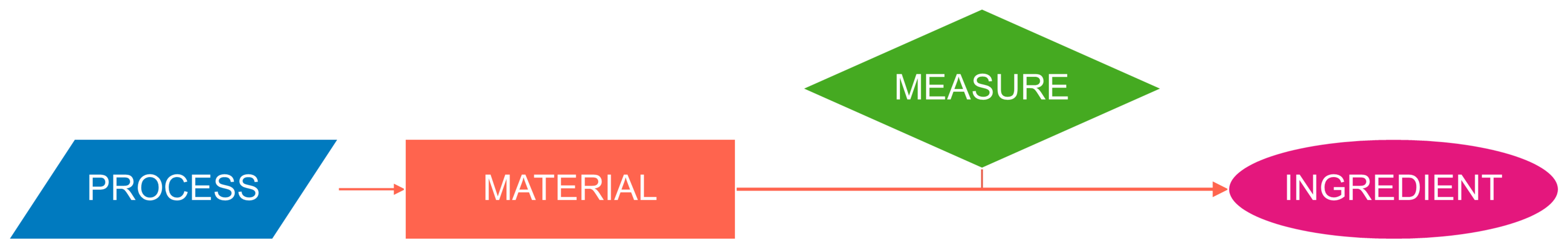

Fig 1. A diagram of the typical nodes used in a typical GEMD data model. Each node contains information pertaining to relevant attributes and is connected by directed edges.

The Material History

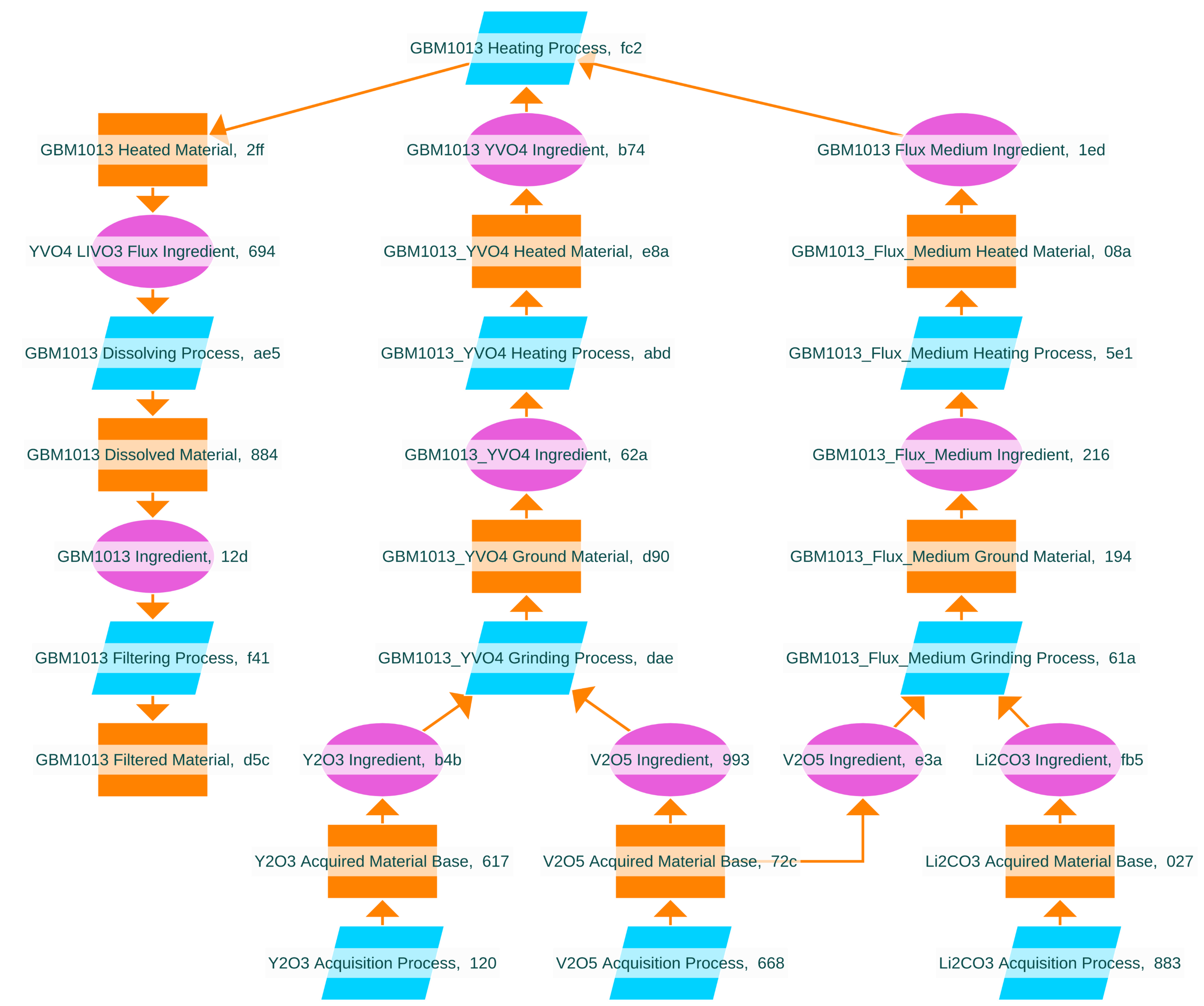

Fig 2. A visualization of the material history of sample GBM1013, a flux growth of YVO_4 crystals. This data structure contains and links all experimental metadata to a characterized end-product, or terminal material.

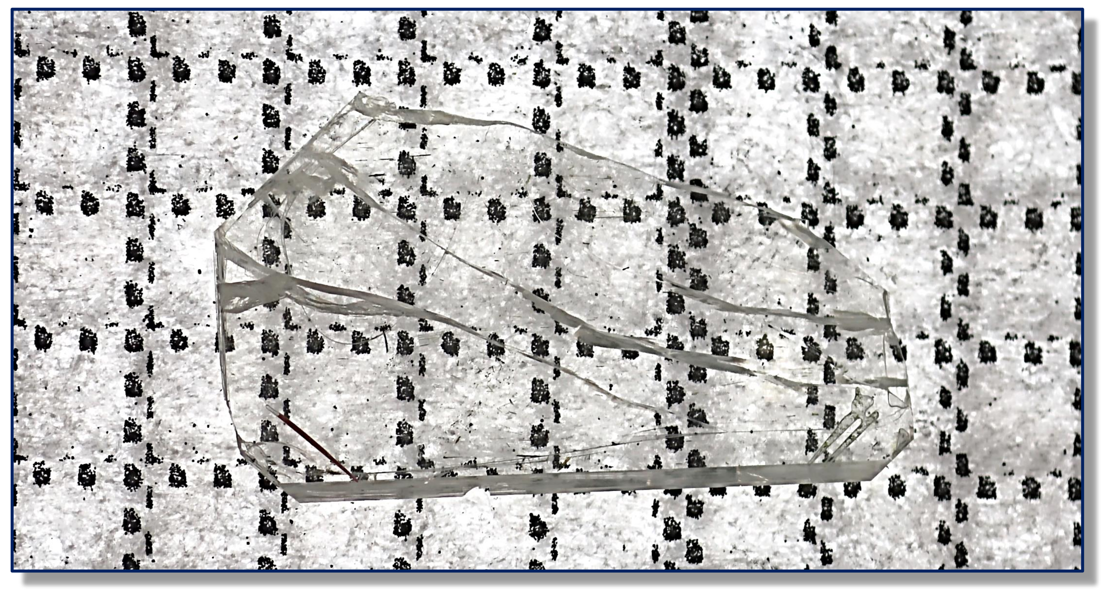

Fig 3. One of the YVO_4 crystals in sample GBM1013, UID d5c above. A crystal of this size and transparency is a promising candidate for facilitating quantum transduction. (1 mm scale)

A Material History, as visualized to the left in Figure 2, utilizes the GEMD model to store all experimental metadata related to the synthesis of a characterized terminal material in a directed acyclic graph. These graphs make it possible to extract and explore detailed information about a given synthesis pathway for later analysis.

A set of Material Histories can be used to construct a database for further exploration. Given a selection of relevant terminal materials, the associated Material Histories become helpful tools for querying entire experiments or individual nodes to find patterns in organic laboratory data. If a Material History database is sufficiently large, the machine-readability of the open data format could be leveraged with the assistance of a graphical neural network model for accelerated discovery.

Data published with Material Histories is ready to be accessed for meta-analysis. This empowers more effective collaboration and data-sharing between scientific institutions and the general public, achieving the goals laid out by the MGI Strategic Plan (2021) and the Nelson Memorandum.

For the purposes of this project, metadata was captured by a variety of methods. Most data was manually recorded in an electronic lab notebook using a series of helper functions. It is also possible to implement live data-streaming from instruments or other sources directly into the model. Once the data was captured, it was processed into alternative formats for further use, including the rendering of visualizations like the one pictured right. More information about the technical execution of these Material Histories can be found in the project's GitHub documentation linked below.

Synthesis and Characterization Methods

In order to collect experimental metadata, YVO_4 syntheses were attempted by flux, laser-diode floating zone (LDFZ), and hydrothermal methods.

Synthesis under mild acidic hydrothermal conditions was not successful as crystallization was not observed for any trial. The author speculates that this was the result of instrument failure.

Fig 4. $LiVO_3$ flux matrix containing YVO_4 crystals.

Flux synthesis (pictured left) produced a variety of crystals, ranging from needles on the scale of microns to larger plates of several mm, as in Figure 3 (above right).

LDFZ synthesis (pictured right) produced several large, cylindrical crystals up to 50mm in length. These crystals were rather clear and demonstrated strong grain selection.

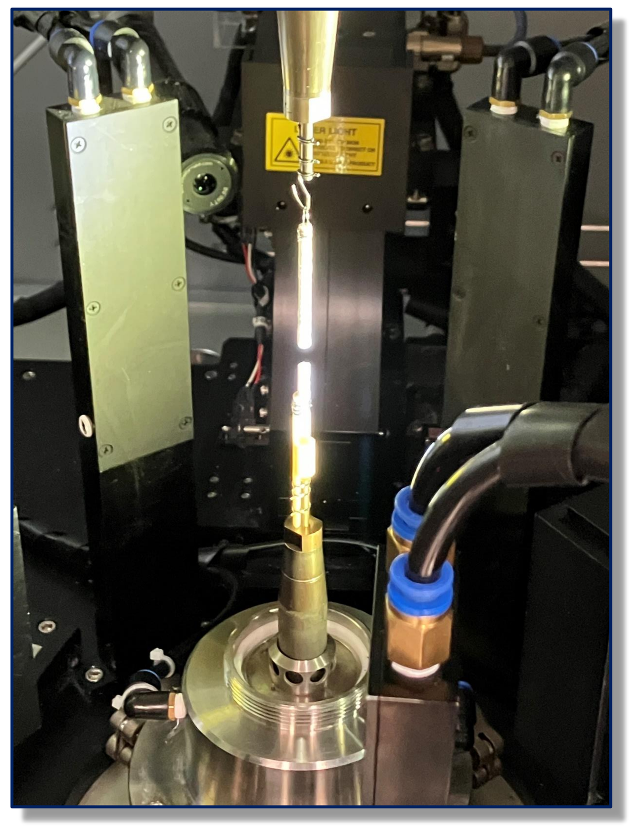

Fig 5. YVO_4 rods being prepared for an LDFZ synthesis.

Powder X-Ray diffraction spectra were captured for each synthesis in order to confirm the composition and identify the crystal structure of each sample.

Additional characterization techniques could have included Scanning Electron Microscopy or Electron Paramagnetic Resonance to study the topology and electronic structure of the sample, respectively.

Additional Resources

GITHUB

RESOURCES

Acknowledgements

Special thanks goes to David Elbert and Brandon Wilfong for their guidance and support for this project. Additionally, the author would like to thank Ali Rachidi for his advice and technical assistance. Finally, a large thanks is owed to Tyrel McQueen, Jim Overhiser, and the rest of PARADIM for their continued support and facilitation of this research.