Using the Graphical Expression of Materials Data (GEMD) model to instantiate experimental metadata related to the synthesis and characterization of Yttrium Orthovanadate.

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ABSTRACT: In the shifting landscape of materials research towards data-driven approaches, the need for robust data sharing policies is paramount. This study addresses this need by introducing the Graphical Expression of Materials Data (GEMD) model. The model is employed to create Material Histories, encapsulating comprehensive experimental metadata for Yttrium Orthovanadate (YVO4) syntheses using various methods.

INTRODUCTION

As the demands of materials research and design shift from traditional methods towards data-driven approaches, it is essential that laboratories develop robust policies and procedures to facilitate data sharing. In 2011, the White House Office of Science and Technology Policy (OSTP) spearheaded the federal interagency Materials Genome Initiative (MGI) to promote the acceleration of materials research. In 2021, the MGI published a strategic plan[3] which establishes a framework for the development of a national materials data network and preparation of the future research workforce to leverage such a resource. In 2022, the OSTP Acting Director for Science and Society Dr. Alondra Nelson released a memorandum[4] calling for the prompt adoption of public data sharing policies by federally funded research laboratories.

Shared data is most effectively leveraged when researchers can establish its context and value from rich metadata. For those interested in the design and synthesis of novel materials, experimental metadata serves this purpose. Experimental metadata includes information pertaining to experimental procedures and parameters, environmental conditions, instrument and reagent details, and provenance. Capturing and instantiating experimental metadata requires rigorous laboratory procedures and a robust schema.

This study serves as a proof-of-concept for the end-to-end implementation of the Graphical Expression of Materials Data (GEMD) model, co-developed by PARADIM and Citrine Informatics. The GEMD model allows for the development of a Material History which contains all experimental metadata related to a characterized terminal material.

In this study instantiation procedures were developed and utilized to capture syntheses of Yttrium Orthovanadate (YVO_4), pictured below in Figure 1. YVO_4 is a colorless, transparent crystal with a tetragonal zircon structure with traditional applications in optics.

Partners of PARADIM are interested in YVO_4 for its potential as a host material of Yb^{3+} for microwave-optical quantum transduction.

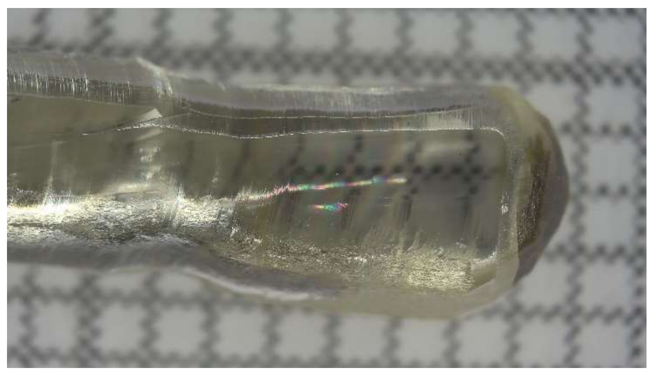

Figure 1. A YVO_4 single crystal synthesized via floating zone method. Scale = 1mm.

METHODOLOGIES

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

Synthesis under mild acidic hydrothermal conditions was not successful as crystallization was not observed during any trial. Parameters and conditions were selected based on the work of Byrappa et al[1].

Flux synthesis in Lithium (III) Vanadate produced a variety of polycrystals, ranging from needles on the scale of microns to larger plates of several millimeters, as pictured in Figure 2 below. Parameters and conditions were selected based on the work of Erdei et al[2].

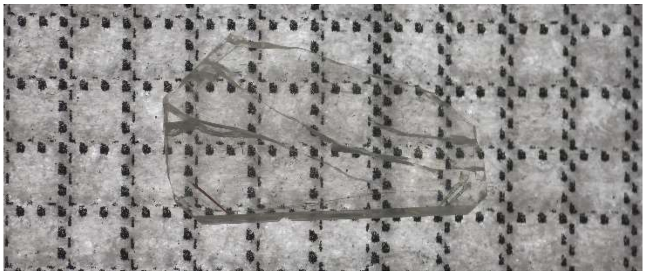

Figure 2. Plate crystal of YVO_4 synthesized in $LiVO_3$ flux medium. Scale = 1mm.

LDFZ synthesis produced large, cylindrical single crystals up to 50mm in length. These crystals demonstrated good clarity and strong grain selection. In addition to pure YVO_4, several samples were made with nominal 1% Yb^{3+} doping, as pictured in Figure 3 below.

Figure 3. Single crystal of $Yb:YVO_4$ synthesized via laser-diode floating zone. Scale = 1mm.

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

As each synthesis was conducted, experimental metadata was captured using a Jupyter-based electronic laboratory notebook. This notebook used the GEMD Python library to store captured information in the GEMD model. A detailed breakdown of the technical execution of instantiation, as well as all data captured this way, can be found here.

The model stores materials data as nodes in a directed acyclic graph (DAG). GEMD node types include materials, processes, measurements, and ingredients as depicted in Figure 4 below. Nodes can have associated property, condition, and parameter attributes as well as any number of tags and unique identifiers. A graph that describes the complete synthesis of a material is referred to as a Material History.

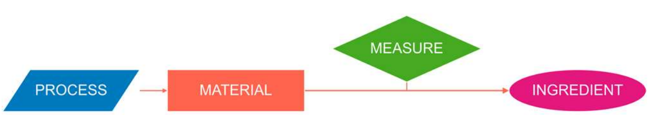

Figure 4. A diagram of the typical nodes used in a typical GEMD data model. Each node contains information pertaining to relevant attributes and is connected by directed edges.

DISCUSSION & FUTURE WORK

Material Histories were successfully generated for a series of YVO_4 syntheses using the GEMD model. These graphs encapsulate a detailed record of the experimental metadata associated with each synthesis pathway. The model provides a systematic and organized representation of the sequential processes and ensures the preservation of information flow, enabling efficient retrieval and exploration. Below in Figure 5 is a visualization of the data structure for a Material History.

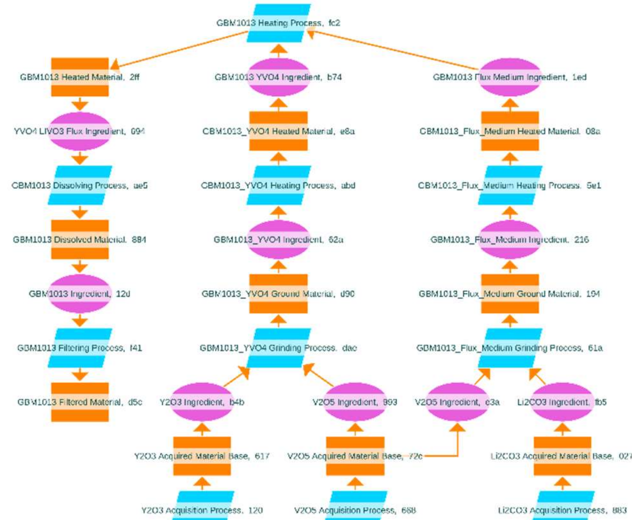

Figure 5. The material history of sample GBM1013, a flux growth of YVO4 crystals. This data structure contains and links all experimental metadata to a characterized end-product, or terminal material.

The collection of material histories can serve as the foundation for constructing a comprehensive database for materials research. By assembling a diverse set of material histories, it is possible to establish a resource that enables researchers to query and investigate entire experiments or granular processes. This capability facilitates the identification of patterns and correlations in laboratory data, enhancing the potential for informed decision-making and hypothesis generation in materials design.

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