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Extended Abstracts

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FDOs and Materials Science and Engineering

Zachary Trautt

Material Measurement Laboratory, National Institute of Standards and Technology, USA

Correspondence: zachary.trautt@nist.gov

Abstract. This lightning talk summarizes past and future work towards FAIR Digital Objects (FDOs) within the materials science and engineering (MSE) community. This talk will: (1) present a view of how past and future efforts could align with the FDO vision, (2) use x-ray diffraction, a materials characterization technique, to illustrate the concepts of Types, Objects, and Operations, and (3) discusses how the same paradigm could be applied to current efforts and systems for (meta)data interoperability.

Keywords: FAIR Digital Objects, Materials Science and Engineering, X-Ray Diffraction

FDOs and Materials Science and Engineering

MSE represents one of the most complex use cases for adopting the FDO vision. Firstly, the domain has strong commercial interests. Thus, practitioners often mix publicly available data with internal proprietary data. Secondly, where other domains have simple sources of data and metadata (e.g., geospatial coordinates), MSE involves complex and multidimensional data and metadata. For example, a new material can be simulated via high-performance computing (HPC) or synthesized via an experimental methodology. Methods vary considerably and span several orders of magnitude in time and spatial dimensions. The data and metadata linked to a newly synthesized material may include the entire processing history of the material and a set of measurements to determine chemical composition, structure, and various mechanical or functional properties. This complexity helps explain why progress toward FAIR data has remained slow and siloed within the international MSE community.

Several efforts may help inform the adoption of the FDO vision within MSE and may serve as platforms to promulgate the FDO vision. These efforts include:

- Harmonised terminologies and schemas for FAIR data in materials science and related domains Working Group[1] — This recently proposed Research Data Alliance (RDA)[2] group could incorporate the FDO vision into its work and recommendations.
- Materials Research Data Alliance (MaRDA)[3]—This grassroots network was recently established to serve the data-driven MSE community. Although there is no formal relationship between RDA and MaRDA, some of its operations are modeled after the broader RDA.
- Open Databases Integration for Materials Design (OPTIMADE)[4]—This consortium aims to make materials databases interoperable by developing a specification for a common REST API. The current specification and adoption are best suited for atomistic methods and crystallographic data. Currently, more than 20 repositories support the API specification[5].

- RDA International Materials Resource Registries WG[6]—Representatives of the MSE formed this group, developed an XML-based metadata schema, and worked to deploy two U.S.-based registry instances[7,8], which exchange metadata via the OAI-PMH protocol [9].
- RDA Materials Data, Infrastructure & Interoperability IG[10] — Representatives of the MSE formed this group to organize and coordinate the development of data exchange protocols.
- RDA Data Type Registry (DTR) Working Group[11]—Representatives of the MSE engaged in this effort, using X-ray diffraction as an example use case to consider the role of Types and Operations within the community[12].
- Other RDA Groups that impact FAIR for MSE include Machine Learning[13], Physical Samples[14], Instruments[15,16], Software[17], and many others.

Using x-ray diffraction as an example to conceptualize the FDO paradigm, a θ-2θ Diffractogram could be considered an FDO Type definition, an example use case in the DTR demonstration project[18]. The measurement of a specific region of a material sample will generate an FDO (with links to other FDOs describing the sample and instrument). An FDO Operation could be a request for a reduced representation of the data that reports peak locations within the data. Furthermore, the FDO paradigm could be leveraged as a layer above existing exchange protocols, where an FDO Type could describe records in a resource registry or an OPTIMADE repository, and a request to an OPTIMADE or OAI-PMH endpoint could be represented as an FDO Operation.

Moving forward, our efforts are focused on spreading awareness of the FDO paradigm and making future MSE recommendations/specifications consistent with the FDO specifications.

Competing Interests

The authors declare that they have no competing interests.

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