

Domain level ontology design: DISO and MDMC-NEP Prov

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Dislocation Ontology (DISO)

Introduction

Dislocation is a defect type in metals that determines important material properties, e.g., strength and ductility. Together with materials scientists, HMC supports and co-develops the dislocation ontology (DISO). DISO is a domain ontology that defines the concepts and relationships related to dislocation in crystalline materials.

Ontology Development

We interviewed domain scientists for domain exploration. Together, we conceptualized and formalized the domain knowledge into an ontology. A list of competency questions to evaluate ontology is available [here](#).

Ontology

Most crystalline materials contain many defects and the dislocation is one of various defect types. **Distinguishing the different abstractions** of the dislocation is important to conceptualize classes and their relationships.

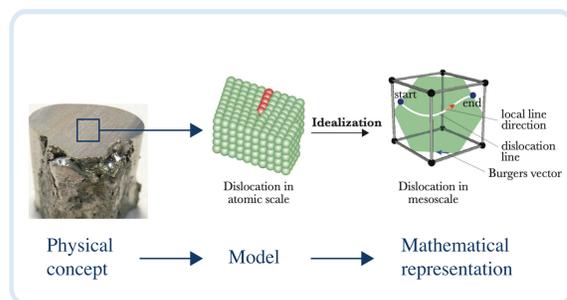


Figure 2: The conceptualization process of domain description in dislocation ontology. We distinguish the physical, model, and mathematical/numerical representation concepts that define classes and relationships in DISO.

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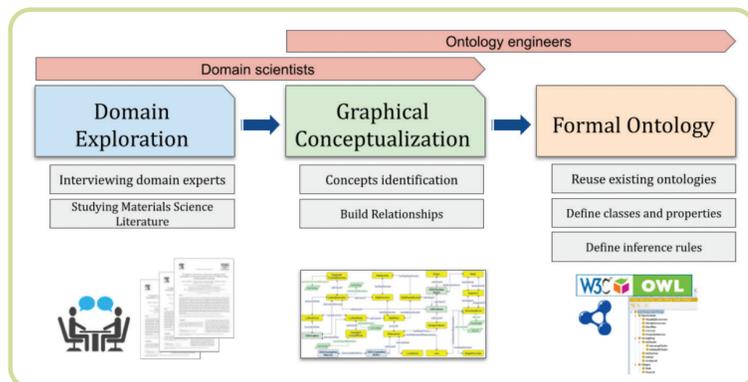


Figure 1: The workflow of the dislocation ontology development is illustrated, including the main phases, subprocesses, and roles involved in the whole process.

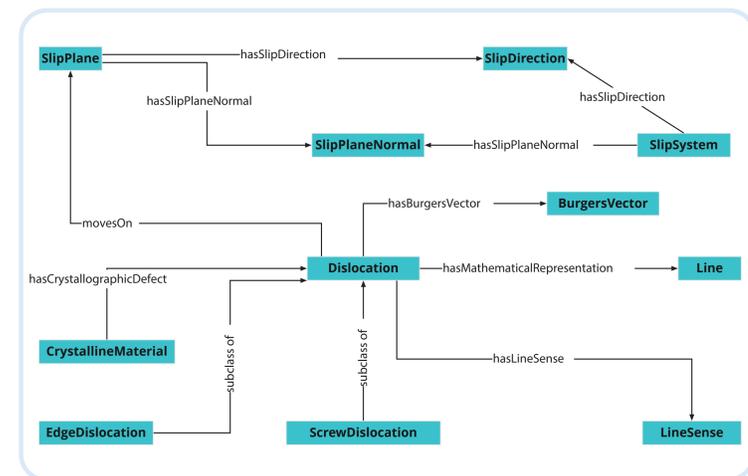


Figure 3: The result of the graphical conceptualization will be formalized into the ontology. Formalization means transferring the knowledge into the language/logic that the computer will understand.

Visit us DISO and MDMC-NEP Prov Github Repository

MDMC-NEP Prov

About

The Joint Lab “Integrated Model and Data-Driven Materials Characterization” (MDMC) of the Helmholtz Association, the Nanoscience Foundries and Fine Analysis (NFFA) Europe Pilot (NEP), EOSC-Pillar and the Helmholtz Metadata Collaboration (HMC) co-developed the MDMC-NEP Prov ontology, which is based on the **MDMC Glossary** and is aligned with **PROV-O**.

Ontology and STM use case

- The ontology contains **high-level provenance information to describe or annotate** the entire experimental workflow/data flow.
- The classes, relations, and properties have been defined **in common** for MDMC, NEP, and EOSC-Pillar.
- The ontology can be **potentially used/extended** to other materials science domains.
- The first application use case is on **Scanning Tunneling Microscopy (STM) experimental workflow**.

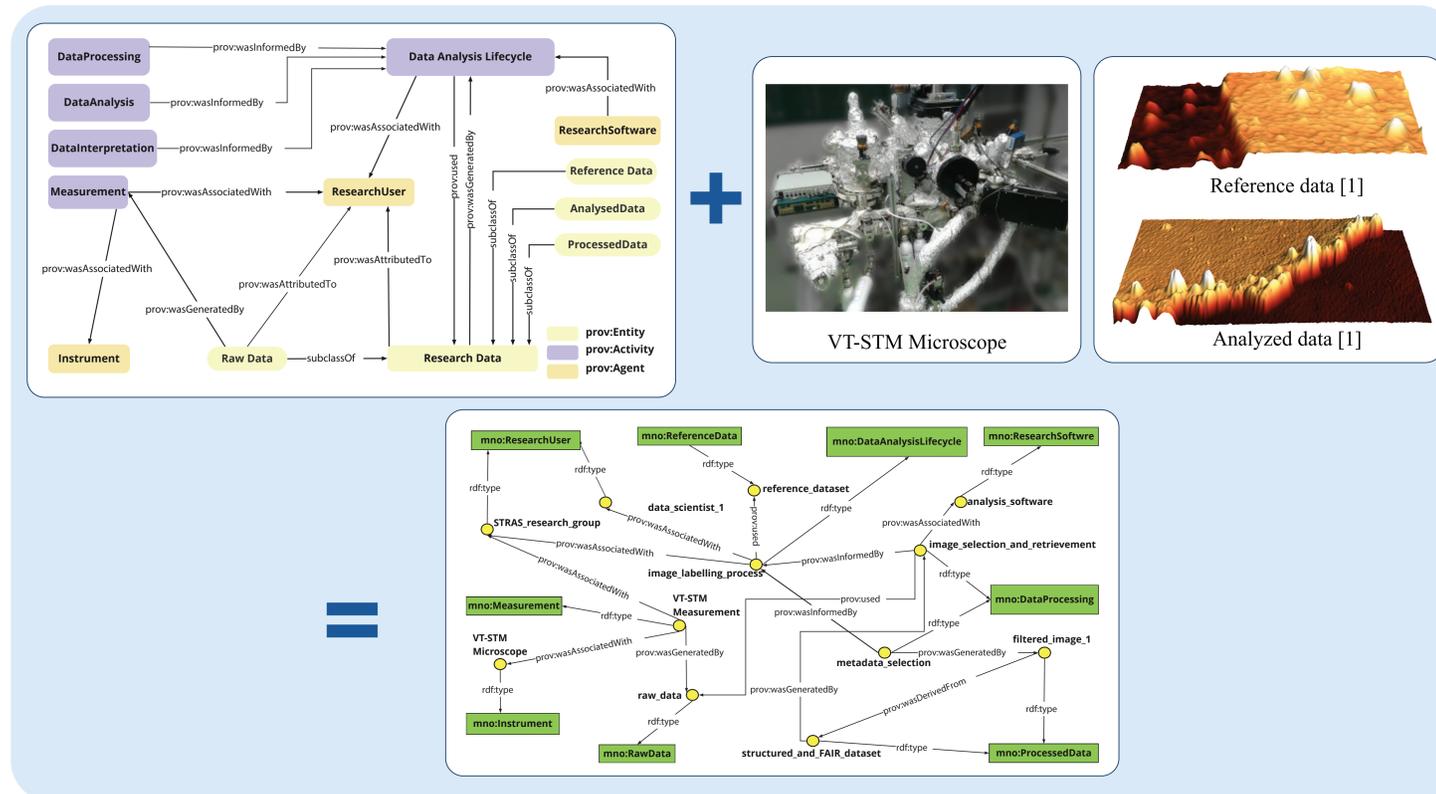


Figure 4: The mapping of the STM use case (top right figure) with the MDMC-NEP Prov Ontology (top left figure) results in the ontology instantiation (bottom figure) in the triples format (RDF)/provenance graph. MNO (MDMC-NEP Prov Ontology) is used as a prefix.

References

[1] <https://pubs.rsc.org/en/content/articlelanding/2022/NR/D1NR06485A>

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