DISOS: An ontology suite for modeling dislocations in crystalline materials

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Overview

The dislocation knowledge is explicitly conceptualized and formalized [1]. This will enable machines to understand and analysis dislocation-related data in an efficient manner.

- **Explicit conceptualization** involves the identification of relevant concepts and relations between the concepts along with the explicit definition [2]. These concepts are defined according to **physical concept, model, model idealization**, and **numerical construct** (Figure 1).
- **Ontologies development:** Formal semantics are expressed using semantic web technologies, including RDF, RDFS, and OWL.
- **Stakeholders**: domain scientists as well as ontology engineers.

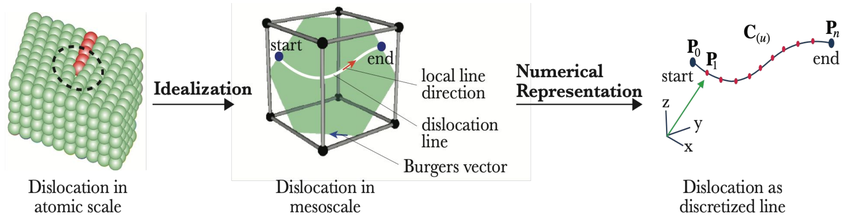


Figure 1. The model idealization represents the dislocation in the mesoscale.

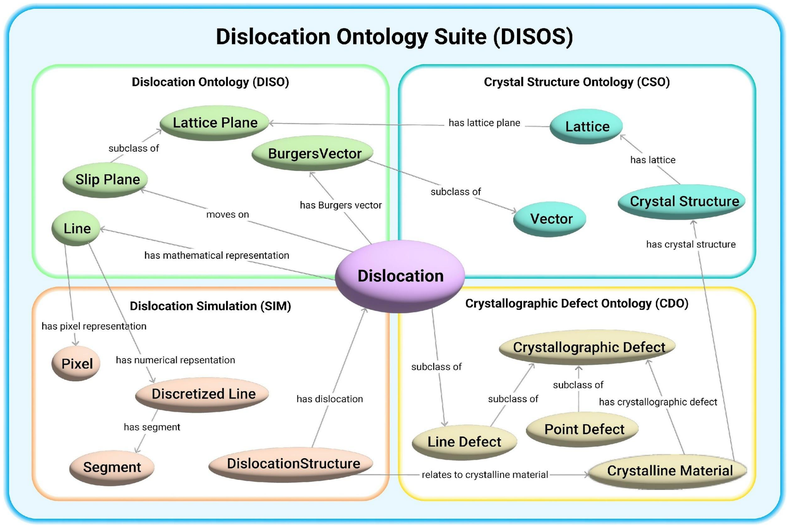
The dislocation ontology suite (DISOS)

The Dislocation Ontology (DISO) [1] represents dislocation-related concepts such as dislocation, Burgers vectors, slip planes, and slip systems.

The Dislocation Simulation Ontology (SIM) models data-related aspects of some simulation frameworks in the context of dislocation simulations.

The Crystal Structure Ontology (CSO) represents crystallographic information needed to describe the dislocation.

The Crystallographic Defect Ontology (CDO) connecting the physical materials entity to the crystal structure and several defects in crystalline materials.



Ontology alignments

Ontology alignment is the process of identifying relations between entities among different ontologies in order to establish connections between them [3]. Currently, DISO is aligned (see Figure 3) with several well-known ontologies:

1. Elementary Multi-perspective Material Ontology (**EMMO**)
2. Materials Design Ontology (**MDO**)
3. Quantities, Units, Dimensions, and Types Ontology (**QUDT**)

Ontology alignment promotes data interoperability between DISOS and domain-related ontologies in materials science and engineering.

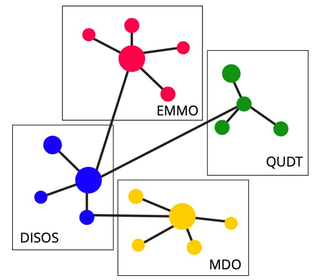


Figure 3. DISOS aligns with several ontologies, e.g., EMMO, QUDT, and MDO

Use cases

Dislocation simulation data

CDO DISO SIM CSO

Modeling discrete dislocation dynamics data. The information collected from the discrete dislocation dynamics (DDD) simulation (see Figure 4) is annotated using all DISOS modules. The DDD data used in this use case is generated through the MoDELib software [3].

Crystal structure data

CSO

Transforming CIF data into linked data. Crystallographic Information File (CIF) data, e.g., Nickel, Aluminium, Tungsten, and Zirconium is annotated using the CSO.

Dislocation microstructure

SIM DISO

Dislocation structure of a virtual dislocation specimen. The dislocation structure is annotated using SIM and DISO. The dislocation structure produced is a virtual specimen of Nickel used by a dislocation dynamics simulation (see Figure 4).

Slip system data

CSO DISO

Crystallographic information of a dislocation structure. The crystallographic information of dislocation data is annotated using DISO and CSO. It includes data of, e.g., slip system and slip direction.

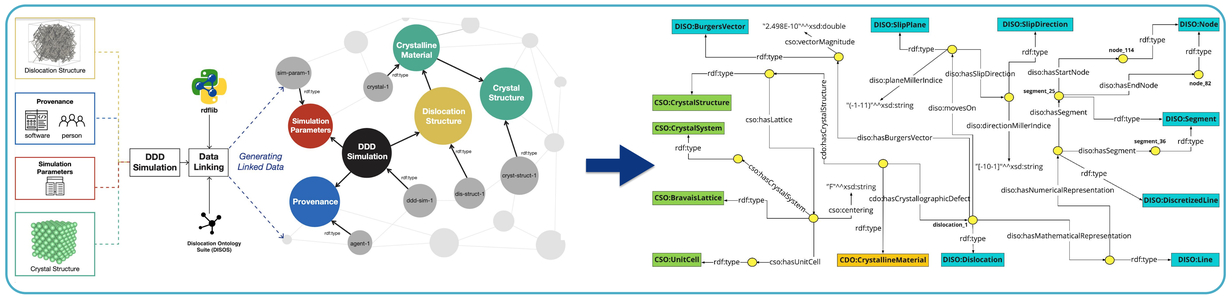


Figure 4. Modeling discrete dislocation dynamics data results in dislocation structure represented as a knowledge graph.

References

[1] Ahmad Zainul Ihsan, Said Fathalla, and Stefan Sandfeld. 2023. DISO: A Domain Ontology for Modeling Dislocations in Crystalline Materials. In The 38th ACM/SIGAPP Symposium on Applied Computing (SAC '23), March 27-March 31, 2023, Tallinn, Estonia. ACM, New York, NY, USA, Article 4, 8 pages. https://doi.org/10.1145/3555776.3578739

[2] Thomas R. Gruber: A Translation Approach to Portable Ontology Specifications. Knowledge Acquisition, 5(2):199-220, 1993.

[3] Marc Ehrig, Ontology alignment: bridging the semantic gap. Vol. 4. Springer Science & Business Media, 2006.

[3] Giacomo Po and Nasr Ghoniem. 2014. A variational formulation of constrained dislocation dynamics coupled with heat and vacancy diffusion. Journal of the Mechanics and Physics of Solids 66 (2014), 103–116. https://doi.org/10.1016/j. jmps.2014.01.012

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DISOS Use Case

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