Contribution ID: **31** Type: **Poster**

DISOS: An Ontology Suite for Modeling Dislocations in Crystalline Materials

Tuesday 10 October 2023 14:30 (15 minutes)

Materials Science and Engineering (MSE) is concerned with the design, synthesis, properties, and the performance of materials. Metals and semiconductors are an important type of crystalline materials that usually have defects. One of the common types of line defects is the "Dislocations"which strongly affect numerous material properties, including strength, fracture toughness, and ductility.

The past few years have seen a significant effort in understanding dislocation behavior at different length scales, using both experimental and simulation techniques. However, there is still a lack of common standards to represent and connect dislocation-related knowledge across different communities. An ideal solution to this problem is to represent this data using a formal language with unique and well-defined concepts that is also accessible to machines. Formal knowledge representation through ontologies allows for data interoperability and sharing between related MSE domains in a machine-readable format, thereby enabling machine actionability.

We develop the Dislocation Ontology Suite (DISOS), an ontology suite that comprises four modules describing scientific concepts of materials, representations of dislocations, and different simulation models in the dislocation domain: 1) the dislocation ontology (DISO) [1] represents dislocation-related concepts such as Burgers vectors, slip planes, and slip systems; 2) the Crystallographic Defect Ontology (CDO) describes the physical entity of crystalline materials and crystallographic defects concepts; 3) the Crystal Structure Ontology (CSO) describes the crystal model/representation and coordinate system, and 4) Simulation Data (SIM) models data-related aspects of some simulation frameworks in the context of dislocation simulations. Furthermore, DISOS is used to describe dislocation-related data (see, e.g., the RDF dataset [2] of dislocation data) with the goal of increasing the interoperability in dislocation use cases. We believe that efforts made are important for establishing FAIR (Findable, Accessible, Interoperable, and Reusable) [3] data in the MSE domains.

References
[1] A. Z. Ihsan; S. Fathalla; Stefan Sandfeld. In The 38th ACM/SIGAPP Symposium on Applied Computing (SAC '23), 2023. https://doi.org/10.1145/3555776.3578739
[2] https://purls.helmholtz-metadaten.de/disos/rdfdata
[3] Wilkinson, M. D. et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci. Data 3:160018 doi: 10.1038/sdata.2016.18 (2016).

Please assign your contribution to one of the following topics

Data interoperability through harmonised metadata and interoperable semantics

Please specify "other" (stakeholder)

In addition please add keywords.

Ontology, Dislocation, Crystallographic Defects, Semantic Web

Please assign yourself (presenting author) to one of the stakeholders.

Researchers

Primary author: IHSAN, Ahmad Zainul

Co-authors: FATHALLA, Said; SANDFELD, Stefan

Presenter: IHSAN, Ahmad Zainul

Session Classification: Poster session

Track Classification: Poster session