

From CHADA to CHAMEO: a reference system for characterisation data management

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1. Introduction

The CHADA (Characterisation Data) template was developed and standardised (CWA) [1] as a common format for documentation materials characterisation, with a view to generality across any type of characterisation method.

In order to provide a machine readable and actionable version of CHADA, the CHAMEO (CHaracterisation METHodology Ontology) [2] has been developed in the NanoMECommons project [3]. CHAMEO includes all terms/metadata of CHADA in a unified, EMMO-based semantic model that describes the classes of metadata and how concepts relate to one another, i.e. it provides context and meaning.

CHAMEO is the overarching reference for sub-domain and application ontologies. It has already been applied to areas ranging from nanomechanical characterisation (nanoindentation, FIB-DIC) (e.g. of coatings) to partial discharge testing of batteries [4].

2. Towards FAIR documentation of characterisation experiments

The CHADA document template has a structure of sections with generic guidelines to drive the users to providing information about materials characterisation experiments. This template has the goal to provide a standard format, but the generated documentation is only human readable. Though there are indications on how to fill the template, when collecting CHADAs from different operators it arose that different users filled in differently, making the documentation hard to exchange.

To address these issues the CHAMEO ontology has been developed, as a building block towards a machine readable, FAIR documentation of characterisation experiments.

The ontology design process started from the concepts in the CHADA template, then adding classes, relationships and definitions in order to improve the expressivity of the ontology. CHAMEO has been developed and refined through an iterative process involving domain experts on different characterisation techniques, to realise a common framework for the development of technique or application specific ontologies.

Based on EMMO [5] the CHAMEO ontology provides the basic constructs to describe the different kinds of activity that are performed during a characterisation process (e.g. sample preparation, sample inspection, calibration, measurement, data analysis) the experiment itself, which can be simple or a complex workflow, with information about

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the laboratory and the operator, the sample (e.g. material, physical and chemical properties), the hardware involved and the different types of data produced (raw, primary, secondary, characterisation properties).

Ontologies related to specific techniques or applications can be then developed by specialising the basic constructs of CHAMEO. This follows a modular approach for ontology development which also facilitates the interoperability across different characterisation techniques. Figure 1 depicts the modular approach adopted for CHAMEO and CHAMEO-based ontologies.

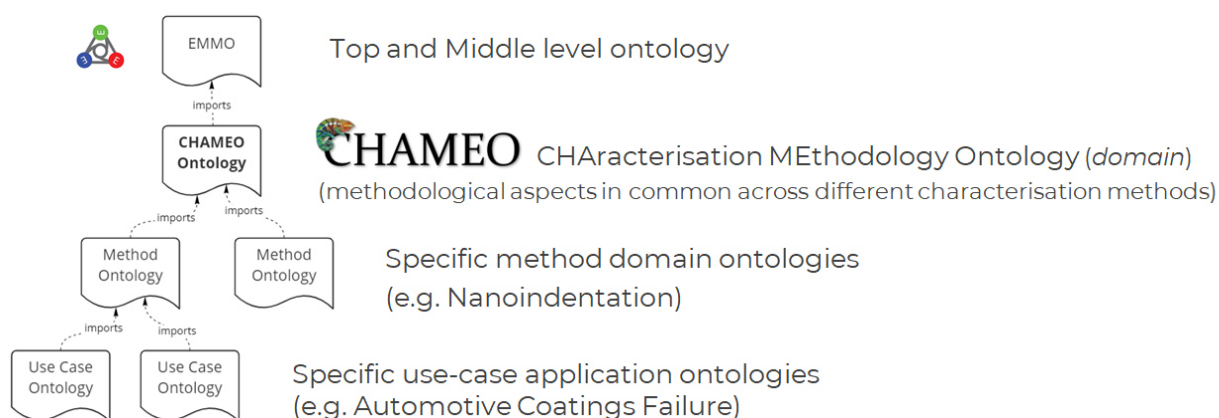


Figure 1 - Ontology design modular approach

The FAIR score of CHAMEO has been measured through the FOOPS validator (https://foops.linkeddata.es/FAIR_validator.htm) and is 92%.

3. Conclusions

A reference ontology for all fields of characterisation has been developed. It provides the basis for curated metadata, harmonised documentation of materials characterisation protocols and a commons data space that supports queries across currently disparate sub-disciplines.

4. References

[1] Materials characterisation - Terminology, metadata and classification, CEN Workshop Agreement CWA 17815 <https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf>

[2] CHAMEO: <https://github.com/emmo-repo/domain-characterisation-methodology>

[3] NanoMECommons project: <https://www.nanomecommons.net/>

[4] <https://github.com/emmo-repo/battery-testing-ontology>

[5] EMMO: <https://github.com/emmo-repo/EMMO>

5. Acknowledgments

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