An Ontology of Magnetocaloric Materials Research

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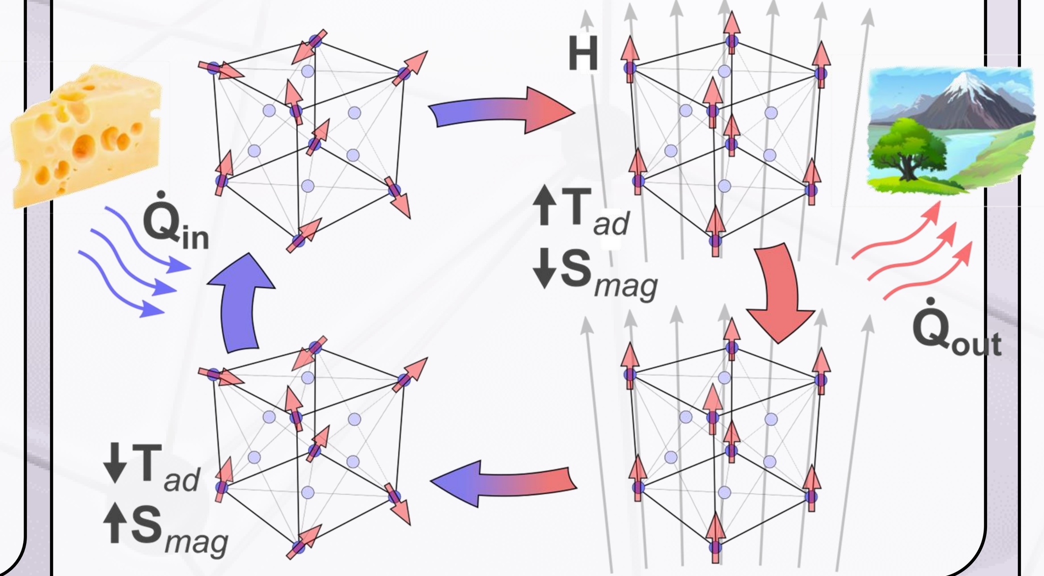
Introduction

Refrigeration based on the magnetocaloric effect (MCE) can contribute to energy-saving, environmentally friendly cooling in private households or industrial application [1]. The cooling is based on heat release or uptake during a phase-transformation of the materials that can be controlled by a magnetic field. This process could replace conventional compression-based refrigeration, which often rely on environmentally harmful refrigerants [2]. DiProMag seeks to digitalize the process chain from theory, simulation and experiment to prototypical applications. The Heusler alloy Co_2CrAl is examined as a model system for potential application in magnetic cooling. OTTR templates are used for the acquisition and semantic representation of knowledge in the development of an ontology. The ontology and additional unstructured data will be used to train a vector space that is analyzed concerning analogies to gain new insights and hypotheses.

What's Magnetic Cooling?

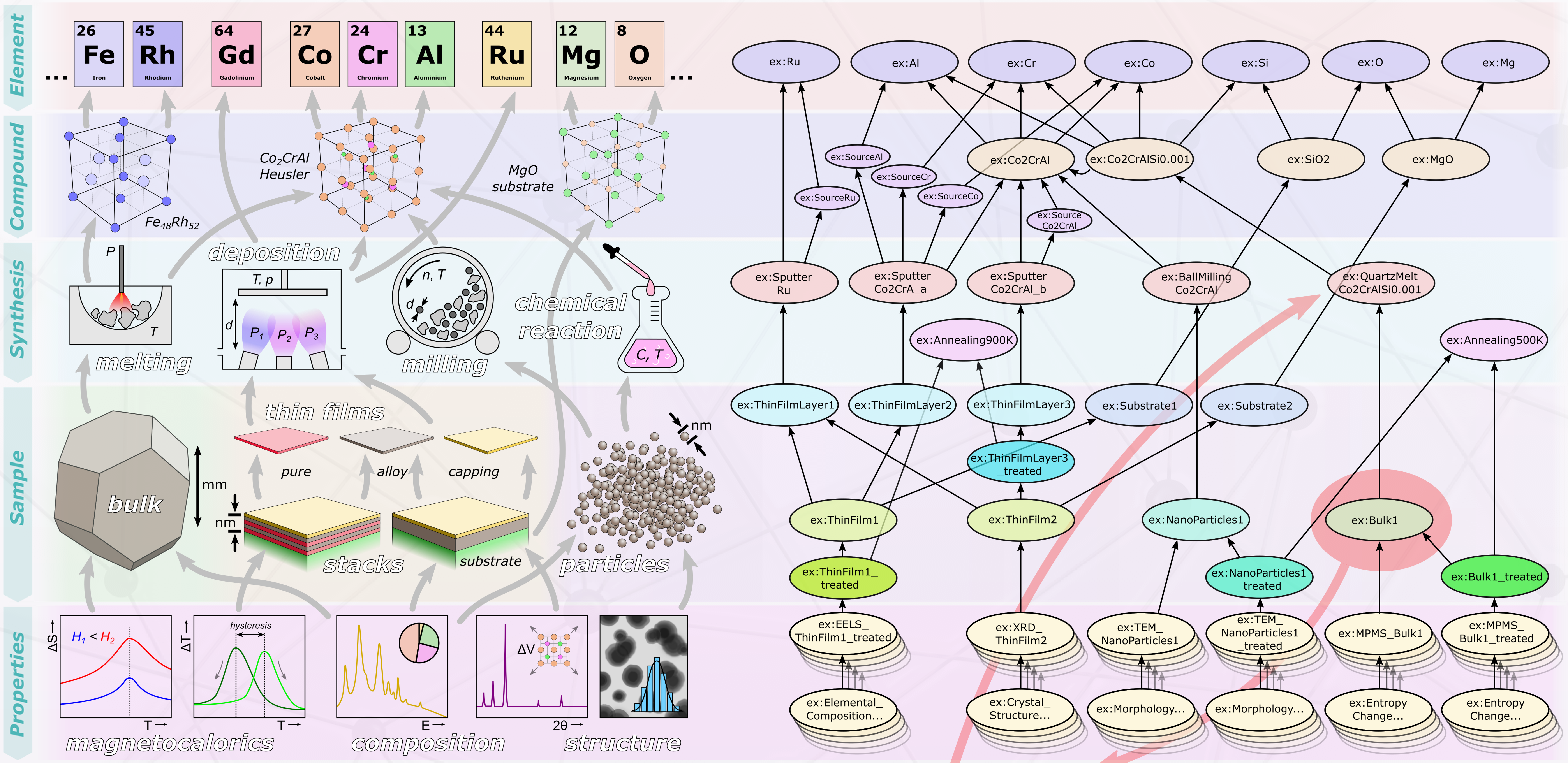
The MCE results from magnetic entropy change during a magnetic phase transition and causes adiabatic temperature change. It is sensitive to material composition [3].



What's an Ontology?

An ontology is a structured representation of knowledge with formal naming of concepts and their relations. They allow machines to retrieve data and allow logical reasoning and machine learning. A template-based (OTTR) [4] approach is used to abstract from raw ontological data, which helps to reduce complexity and facilitates understanding and involvement of domain experts in the ontology development. Ontology engineers and domain experts collaborate to design templates, which are translated to „ontological“ data.

Ontology of Magnetocaloric Materials



The developed ontology models all information along the scientific workflow in the field of magnetocalorics in OTTR templates. The templates are referring to each other according to their relations and positions in the workflows in an hierarchical structure. Templates of measurement results and parameters reference their respective samples. Sample templates reference the respective synthesis method, which in turn references a compound, which is ultimately composed of chemical elements.

Referencing is upward in the diagram (direction of the arrow) and the workflow is downward.

Each template contains entries for parameters, conditions, and evaluations, thus representing a complete semantic description of the scientific workflow. The templates contain documentation that serves as an instruction manual.

Exemplary template for a bulk sample: dpm:SampleBulk

```
ottr:IRI ?sample = dpm:BulkSampleLC20220916a,
NEList<pmdco:Process> ?production_steps =
(dpm:SynnthesisQuartzMeltBulkSampleLC20220916a1000a)
xsd:string ?sample_code = "LC20220916a"^^xsd:string, dpm:Compound
?intended_compound = dpm:Co2CrAl,
NEList<dpm:Element> ?elements = (dpm:Co, dpm:Cr, dpm:Al),
NEList<xsd:float> ?purities_unit_percent = ("0.999"^^xsd:float,
"0.9996"^^xsd:float, "0.998"^^xsd:float),
NEList<dpm:Shape> ?shapes = (dpm:pieces, dpm:flakes, dpm:pieces),
NEList<xsd:float> ?target_masses_unit_kg = ("0.00239516"^^xsd:float,
"0.00105661"^^xsd:float, "0.00054829"^^xsd:float),
NEList<xsd:float> ?actual_masses_unit_kg = ("0.0023952"^^xsd:float,
"0.00105659"^^xsd:float, "0.00054831"^^xsd:float),
NEList<xsd:float> ?mass_deviations_unit_kg = = ("0.0000004"^^xsd:float,
"0.00000002"^^xsd:float, "0.00000002"^^xsd:float), xsd:float
?overall_weight_unit_kg = "0.004"^^xsd:float,
```

At the most basic level, the ontology can be used as a very thorough lab book. The structured digitization of the workflow makes much information that previously went unnoticed accessible for data analysis. The structured information can be screened for any specific content and analyzed for hidden correlations to generate new insights and hypotheses.

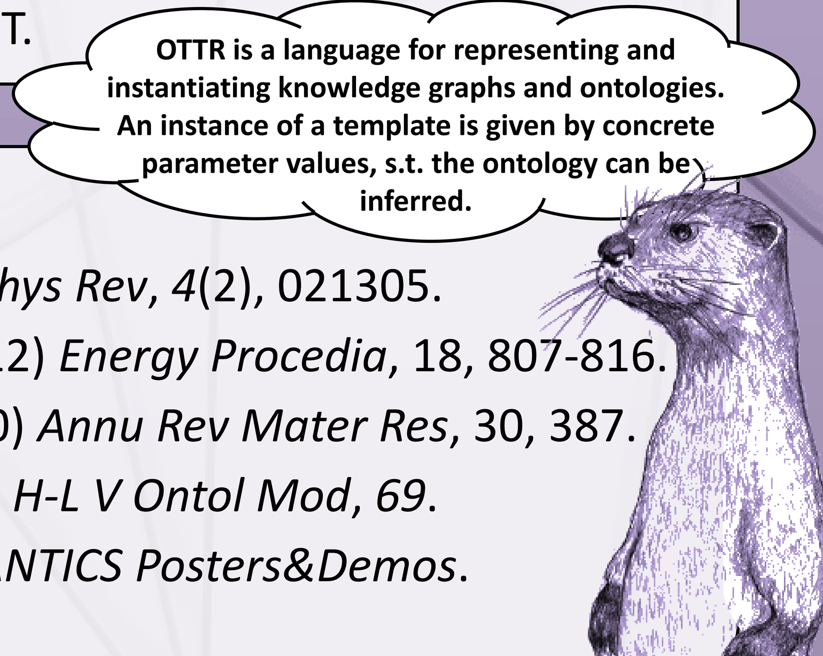
DiProMag takes a holistic approach, addressing all aspects of magnetocalorics and integrating them into the onotolgy - from theory, simulation and experiment to prototypical applications.

The focus of the project is on the advancement of Heusler alloys, with Co_2CrAl serving as the first promising model system (see Diagram) that exhibits a strong first-order phase transition in the vicinity of RT.

Outlook

DiProMag is part of the Platform Material Digital, which seeks to advance the digitalization in material science. The Platform promotes collaboration and ensures interoperability with ontologies from similar projects by involving established ontologies and by reusing their classes and properties.

Published research and ontologies mirror how materials are synthesized, characterized, and applied. Our goal is to automatically extract data from research articles to infer new knowledge. For this, we learn a joint vector space of textual and ontological data on which data science mechanics are applied. The vector space has already been shown to contain real physical knowledge not explicitly present in the data.



References

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[3] Gschneidner et al. (2000) *Annu Rev Mater Res*, 30, 387.
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