Chapter 7

Materials science and ontologies

Jesper Friis, Gerhard Goldbeck, Sylvain Gouttebroze, Francesca Lønstad Bleken, and Emanuele Ghedini

Introduction

Challenges in material innovation towards manufacturing

Materials science is a cornerstone for the development of new manufacturing processes and products. The creation of a new product often starts with materials innovation to improve or replace existing materials. Materials innovation usually includes laboratory experiments, testing, materials characterisation and modelling at various levels of granularity. The research methods in use today have their origins in a wide range of communities, such as chemistry, solid-state physics, materials technology, mechanical engineering, etc. The path from candidate material development to manufacturing of the end product requires multiple consecutive and iterative steps involving multiple fields along the value chain, including additional fields not anchored in materials science, like design, life cycle analysis, safety, sustainability, scale-up and logistics. Each of these fields involves separate communities with their own standards, posing a significant challenge for the exchange of requirements and materials knowledge as well as the efficient use of the information provided.

The key to addressing this challenge lies in interoperability and a robust exchange of knowledge between all stakeholders along the manufacturing path.

Materials digitalisation: the new paradigm

The complexity of the above-mentioned challenge, both in terms of its size and diverse involvement, demands cyber-physical systems and technologies that can support the transition to Industry 5.0 [1] and its focus on greater collaboration and knowledge exchange between humans and machines, involvement of all stakeholders (workers, shareholders, research communities and society) and sustainability. In this chapter, we will focus on materials knowledge and how it can be exchanged between different disciplines involved in the development of new manufacturing products and processes.

DOI: 10.4324/9781032693415-9

The need to coordinate and integrate different communities and their respective methodologies was recognised within the materials modelling community in Europe, leading to the establishment of the European Materials Modelling Council (EMMC) [2] in 2014. A first significant step towards standards and integration was taken by a commonly agreed-upon terminology and classification for materials modelling [3] and a regularly updated roadmap for materials modelling and digitalisation [4]. The roadmap is aligned with the widely endorsed FAIR principles [5] that were coined in 2016, providing guidelines for making data *Findable*, *Accessible*, *Interoperable* and *Reusable*. A similar undertaking was done for materials characterisation, with the establishment of the European Materials Characterisation Council (EMCC) in 2016 [6], which is now closely interacting with and aligned with EMMC. Another important effort for providing a common semantic basis (a human and machine-interpretable language) for materials science and applied sciences, in general, was the initiation of the Elementary Multiperspective Material Ontology (EMMO) [7, 8] in late 2016. EMMO provides a logically rigorous basis for the description of concepts and terminology within applied sciences and a common ground for deep information exchange between experts and the implementation of semantic interoperability.

In 2021, the Advanced Materials 2030 Initiative [9] was initiated with the Materials 2030 Manifesto [10] and one year later followed up with the Materials 2030 Roadmap [11] on how to address the needs for a strong European ecosystem for materials to drive the green and digital transition. The roadmap highlights materials digitalisation as a key priority for meeting the needs for sustainability and expectations from society. Figure 7.1 shows the four prioritised topics within materials digitalisation for accelerating

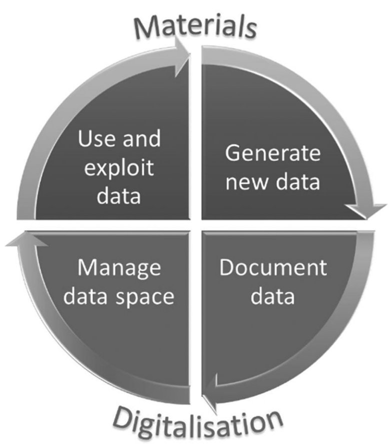

Figure 7.1 The four priority topics to achieve the data life cycle of advanced materials. From Ref. [11].

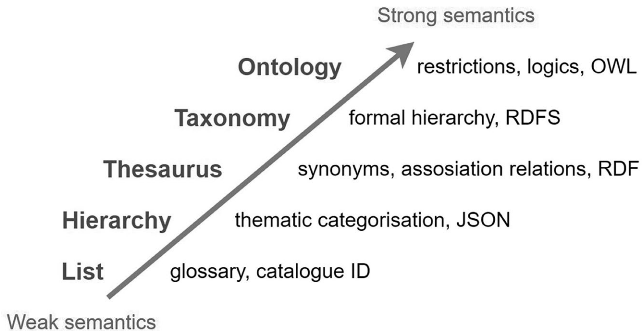

Figure 7.2 Illustration of Semantic Knowledge Organisation (dashed line indicates the limit to enabling semantic interoperability). Adapted from Ref. [12].

the design and use of advanced materials by creating efficient pathways for harvesting and exploiting relevant data. These priorities rely on the efficient exchange of materials knowledge between different stakeholders.

Path towards a solution: semantics and interoperability

Semantic knowledge organisation refers to the organisation of information, providing not only data but also meaning and logic at some level of detail. The level can range from a controlled vocabulary for representing the types of entities in a given domain via a thesaurus and taxonomy (hierarchical classification) to a fully-fledged ontology, as illustrated in Figure 7.2.

We define *compatibility* (from Latin cum = with and pati = to suffer) as the ability of two or more systems to establish a one-to-one connection between them, usually due to strong similarities in their internal representations that facilitate mutual understanding (e.g. for software, this usually happens when systems are parts of a set of tools provided by a common developer) (Figure 7.3b). In a compatibility scenario, systems are fully aware of the type and identity of the other connected systems.

We define *interoperability* (from Latin inter = between and operari = to work) as the ability of two or more systems to exchange information between them through a common representational system to perform a complex task that cannot be done by each single system alone. The presence of a common representational system provides the highest level of generalisation and replaceability and means that no privileged one-to-one connection between two system types should be implemented within the interfaces (Figure 7.3a). In principle, in an interoperability scenario, one system can ignore the details about other systems.

In software systems, compatibility is typically achieved by means of defining and adhering to particular formats or syntaxes; hence, it is also referred to as "syntactic interoperability". In contrast, interoperability as defined

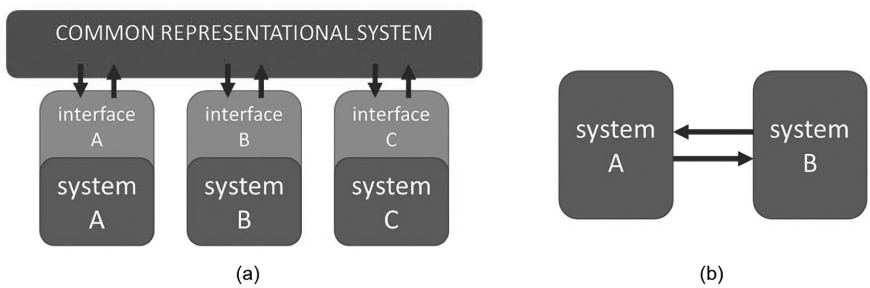

Figure 7.3 Interoperability (a) vs compatibility (b).

above is associated with so-called "semantic interoperability". Most systems today operate at lower levels, i.e., they are compatible due to syntactic interoperability.

At the highest level of abstraction, we find interoperability environments enabling interactions at the human level – between scientific communities or experts belonging to different fields. Such interoperability/integration is achieved by establishing a common "language" (i.e. a common vocabulary, terminology and standardised classification) covering various communities and sub-disciplines that can be used to represent the information. A common language understood by each member of the scientific community will enable effective information exchange.

In Section "An ontology for material science", ontologies are presented in general, including the needs for materials science and a brief introduction to EMMO. Section "Application of ontologies for materials science" shows some applications of ontologies for materials science, starting with the general case of data documentation and followed by some application examples. Finally, Section "Further perspectives" highlights further perspectives.

An ontology for material science

What is an ontology?

An ontology is a formal representation of knowledge that describes the concepts and relationships within a specific domain. Ontologies help to standardise the representation of knowledge within a particular domain and thus facilitate communication and interoperability between different systems and applications. They provide a shared and commonly accepted formalisation of concepts, allowing the knowledge to be understood by experts of different disciplines and by automated systems that can be the basis for artificial intelligence (AI) or big data applications. This can be achieved at different levels of the semantic spectrum using systems that span from lists of terms to complete and decidable logical systems at the ontological level (Figure 7.2).

Ontologies are commonly used in computer science and artificial intelligence applications, such as semantic web technologies and knowledge management systems.

Formally, an ontology consists of classes (representing the concepts), individuals (specific instances of a concept representing a concrete object) and relations (for example, properties) between them, as shown in Figure 7.4a. In addition, can ontologies contain axioms, which are facts or statements that are asserted to be true in the domain being described, as well as rules that define how the classes and properties can be used together. Each class, individual or relation in an ontology is uniquely identified, typically by an Internationalised Resource Identifier (IRI). For example, the IRI http://emmo.info/emmo#EMMO_a4d66059_5dd3_4b90_b4cb_10960559441b uniquely identifies the concept of manufacturing in EMMO. Figure 7.4b shows a simple example of an ontology and how it relates to real-world entities. In this case, the real-world objects are a specific aluminium microstructure and one of its properties, its yield strength, as obtained from a measurement following a given procedure. In the ontological world, individuals

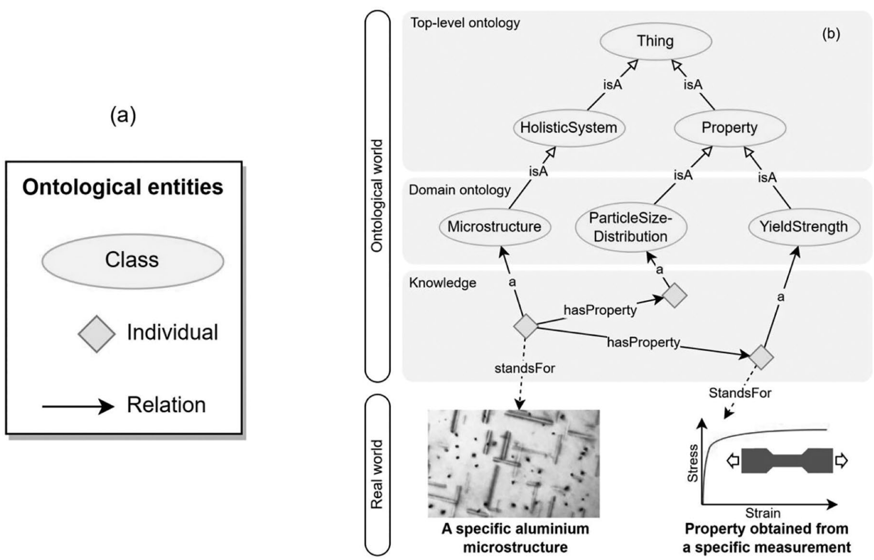

Figure 7.4 (a) ontological entities. (b) an example of an ontology and how it relates to real-world entities. The arrows in (b) have different meanings; the arrows with empty heads represent sub-class relations (rdfs:subClassOf), the arrows labelled “a” relate individuals to the class they belong to (rdf:type) and the two arrows labelled “hasProperty” are relations between individuals. The two dotted arrows relating individuals to the real world entities that they stand for are not part of the ontological world.

stand for real-world objects and the relations between them. The ontology also provides a strong classification of the individuals in terms of well-defined classes. Formal logic is used to (axiomatically) describe whether an individual of one class also is or cannot be an individual of another class, making it possible to both express complex class dependencies and infer new knowledge from the ontology. Figure 7.4b also illustrates that an ontological system is typically divided into different levels – here simplified to a top, domain and knowledge level. The term ontology is typically used for a consistent set of classes (and axioms) in a given domain. When speaking about the entire ontological representation, including the individuals representing a given use case, the terms *knowledge base* or *knowledge graph* are typically used.

The case of materials modelling

The great diversity of terminology and descriptions of materials modelling has been one of the fundamental challenges in establishing a coherent knowledge representation. A solution emerged as a result of a cataloguing and careful analysis of modelling used in more than one hundred European projects, published in the Review of Materials Modelling (RoMM) [13]. It turned out to be possible to categorise models by four different "entities" (see Figure 7.5).

Materials modelling accordingly involves choosing the level of granularity to describe the material and does this in terms of the behaviour of a set of entities.

It follows that any material can be described by any of the entity types. Also, the scale of the material to be described is, in principle, separate from the entity and its granularity. A manufactured object can be modelled at the granularity of for example components or microstructure.

Having chosen the entity (and hence granularity), the materials model involves a "physics equation", which is based on a fundamental physics

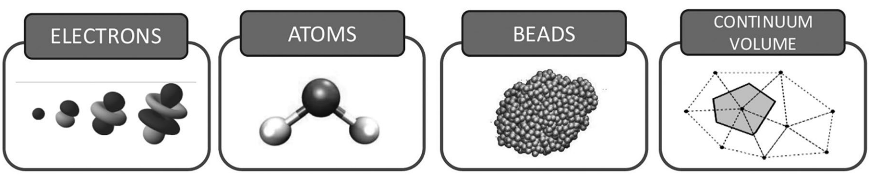

Figure 7.5 Materials model entities: self-contained, internally frozen, structure-less representational units of a material. Standard definitions of electron and atom apply. Bead: a mesoscopic entity consisting of more than one atom (e.g. nanoparticles, grains). Continuum volume entity: a representation of the material bounded in a region of space within which the material is considered to be described by the same set of properties. Originally published in Ref. [8].

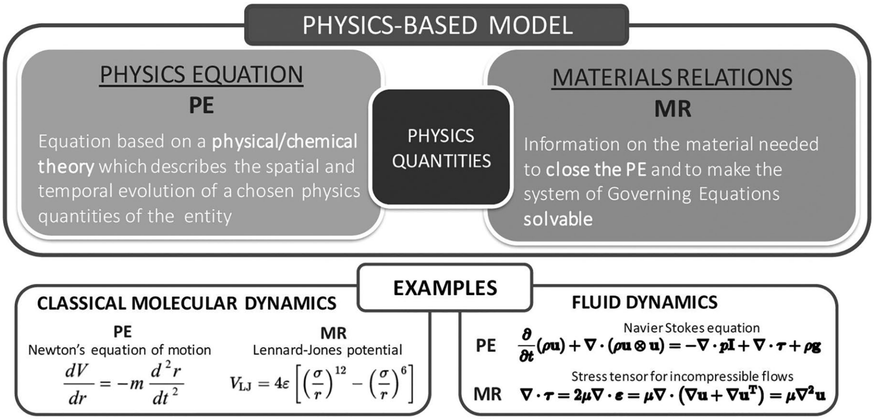

Figure 7.6 A physics-based materials model consists of a physics equation describing the behaviour of an entity and materials relations to make a solvable set of equations. Figure from Ref. [8], which presents the classification work done by Anne F de Baas in the RoMM [13].

theory and defines the relations between the physics quantities of an entity. Well-known examples are Newton's equations, Navier-Stokes equations and the Schrödinger equation. To solve the physics equation, materials-specific equations providing values for parameters in the physics equation are needed. Together with the physics equation, these "materials relations" form a complete set of equations that is solvable, as shown in Figure 7.6.

This classification leads to a great simplification across the wide field of materials modelling. All physics-based models can be categorised by the four entities. For each of the entities, there are about six different physics equations. Of course, much of the knowledge about the specific material is represented in many different materials relations. In atomistic modelling, these are the different potential functions and "forcefields" describing interactions. In continuum mechanics models, materials relations are in fact often referred to as the "materials model". Note that the computational representation of the materials model should be kept entirely separate from the model itself; e.g., finite elements are often used for computational representations of continuum mechanics models. Models are hence classified by their entities (granularity), physics equation and materials relation, neither by the scale of application nor by the computational representation.

The terminology and rigorous classification of materials modelling conducted by EMMC as a CEN Workshop Agreement (CWA) [3] led to a relatively small number of distinct materials models, replacing the former situation of opacity of materials models and simulations that made the field hard to access for outsiders. It also provided a systematic description and documentation of simulations, including the user case, model, solver and post-processor: the "materials MOdelling DAta" (MODA) [3]. It organises information so that even complex simulation workflows can be conveyed more easily, and key data about the models, solvers and post-processors and their implementation can be captured consistently and transparently.

The Elementary Multiperspective Material Ontology (EMMO)

In order to formalise the domain knowledge in materials science, in particular, in an ontology, it is important to have a foundational ontology based on core concepts and perspectives of applied sciences.

These include the scientific view of the world; in particular, there are few "absolutes", e.g., the existence of a universe, and there are basic "rules" that apply everywhere. Patterns and behaviours driven by these rules are uncovered by observation. The latter leads to understanding on a subjective level but not to absolute truths. Similar investigations can lead to different results and have different interpretations. There are accepted scientific laws, for example, regarding elementary entities and their interactions (standard model), cause and effect, conservation of quantities and the fact that matter (fermions) and fields (bosons) are fundamental families of physical entities. An ontology for materials sciences needs to have a straightforward representation of these as well as our understanding of materials in terms of abstract representations of materials structure and the ability to apply granular partitioning into a multitude of separately definable and interconnected levels of size (e.g., micro, meso or macro level items). Furthermore, the close coupling of processes, structure and properties, as well as the need to be able to deal with quantum systems, demands that the spatial and temporal aspects are not separated.

The motivation for creating EMMO as a new foundational ontology for materials stems from the fact that existing ontologies only partially cover the above desiderata. The scope and objectives of EMMO can hence be summarised as follows:

- Common representational framework deeply based in physics, chemistry and materials science.
- Consistent with fundamental theories.
- Ability to represent all materials, chemicals and physical phenomena in a consistent manner.
- Ability to capture all scales and levels of description and zoom in and out in a "hierarchical" manner.
- Capture the strong interrelation between "real world" physical things and their observations/characterisation as well as modelling.
- Ability to deal naturally with changes and processes.

The theoretical foundations of EMMO include:

- **Mereocausality**: A new first-order logic (FOL) theory developed specifically as a foundation for EMMO [14]. It combines classical mereology, the science of parthood relations (part to part and part to whole) with causality (cause and effect). It provides an applied sciences-friendly framework for the representation of spatio-temporal relations among entities. In fact, space and time are not axiomatically assumed in EMMO but rather follow from this underlying theory.
- **Set theory**: The theory of membership. EMMO has a set class representing the collection of all individuals (signs) that represents a collection of items. EMMO makes a strong distinction between membership and parthood relations. In contrast to sets, items can only have parts that are themselves items. For further information, see [15].
- **Semiotics**: The study of meaning-making. It is the discipline of formulating something that possibly exists in a defined space and time in the real world and is used in EMMO to reduce the complexity of a physical thing to a simple sign (symbol) based on Peirce's semiotics [16, 17].
- **Topology**: the study of geometrical properties and spatial (and timewise) relations.

The name *EMMO* should be understood as follows: *elementary* means that EMMO is a discrete ontology, assuming the existence of the smallest possible part; *multiperspective* highlights an important aspect of EMMO – that it is possible to describe the world from different perspectives; *material* (as the opposite of immaterial) emphasises that EMMO is strictly nominalistic, meaning that it assumes that abstracts do not exist. Material also refers to the historical scope of EMMO, aiming at the description of materials and thus covering the needs of physicists and applied scientists.

EMMO development provides a multi-level formalisation of the ontology (i.e. from simple taxonomy to OWL or FOL) in order to be the base for AI applications and data harvesting and interpretations (industry commons and BigData). As shown in Figure 7.7, EMMO is structured hierarchically into

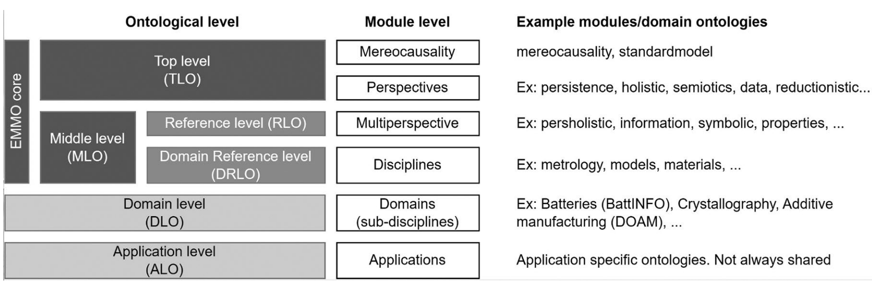

Figure 7.7 The hierarchical structure of ontological levels of EMMO and its domain and application ontologies.

four levels: mereocausality and perspectives at the top level and multiperspective and disciplines at the middle level. Below these, there is a hierarchy of domain- and application-level ontologies.

A full account of EMMO is the subject of a forthcoming publication. Here is just a short outline of the four levels.

Mereocausality level

The fundamental mereocausality theory, where everything is defined (no primitive concepts) according to the causal network between entities whose types and interactions are governed by the standard model and quantum field theory, 4D spacetime arises as a consequence of the combination of mereological fusions and the topological structure of the causal network. The purpose of this level is to provide a consistent theoretical framework anchored in modern physics, providing an unambiguous representation of the world. Users of EMMO can benefit from this foundation without having to learn the underlying theory.

Perspective level

A key feature of EMMO is its ability to represent the world from different perspectives. This is a novel and essential feature for an ontology that has the ambition to express the domain knowledge of all fields of applied sciences. Currently, EMMO includes seven perspectives, as shown in Figure 7.8, but it is possible for users to define their own:

- **Perceptual**: Considers the world as perceived according to human perception mechanisms (visual, auditory, somatosensory, gustatory or olfactory).
- **Physicalistic**: Categorises physical objects only by concepts coming from applied physical sciences.
- **Persistence**: Categorises 4D world objects as they extend in time (process) or as they persist in time (object).
- **Holistic**: Considers each part of the whole as equally important, without the need of a granularity hierarchy (in time or space).
- **Semiotic**: Describes a triadic process in which an interpreter provides a sign for a real-world object. This perspective is based on Peirce semiotics [16] and is about providing meaning. It can be applied to describe processes such as:
  - Measuring the same sample with different devices
  - Providing physical quantities via experiment or modelling
  - Registering feedback from different user experiences
  - Representing different theories for the same phenomenon
  - Applying different names to the same object

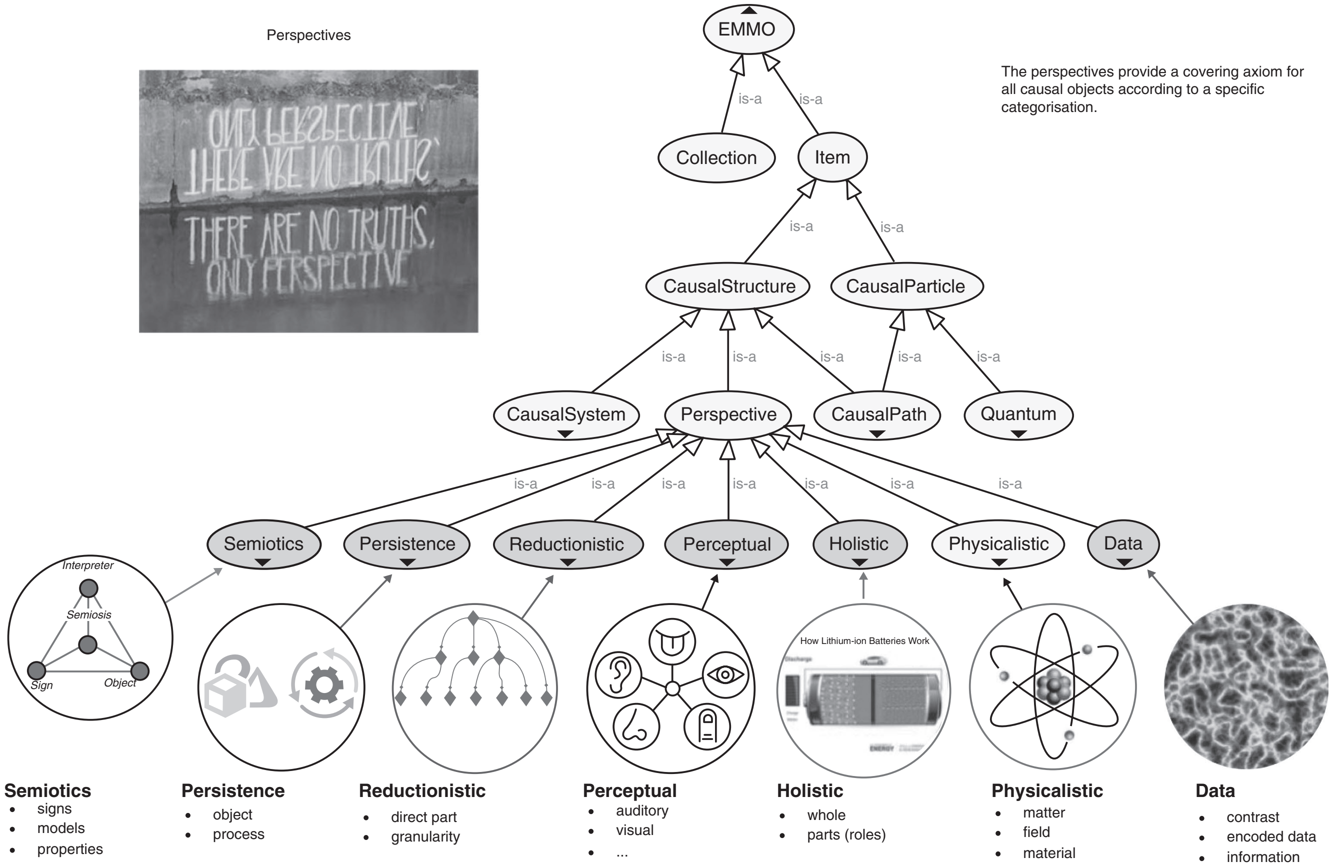

Figure 7.8 The different perspectives currently defined in EMMO.

- Separating what is expected to be (e.g. blueprint) to what will be (e.g. the building)

- **Data**: Categorise data as physical patterns, or gradients, according to their characteristics independently from the carried meaning following the description of information by Luciano Floridi [18].
- **Reductionistic:** Categorises objects according to their granularity relations. This perspective provides the novel notion of direct parthood, allowing a univocal description of granularity levels.

Multiperspective level

Concepts that can be introduced by merging more than one perspective, introducing or not a further level of subjectivity, An example is *information* (usually defined as "data with meaning"), which is the combination of the *data* and *semiotics* perspectives.

Discipline level

The modules at the discipline level provide fundamental concepts limited to specific disciplines. Materials, models and math are examples of disciplines. These are used within many domains and are essential for achieving cross-domain interoperability.

Materials Science ontologies

The motivation for creating an overarching framework for applied sciences is motivated by the heterogeneous nature of the field as well as the strong growth of the field, which calls for some level of harmonisation. A review by Zhang et al. [27] included nine materials ontologies, whereas a more recent study by the OntoCommons project already includes 29 [19]. In addition, there are a number of ontologies in the domain of chemistry [20, 28]. EMMO is able to address the needs for a semantic description that covers the wide physical sciences integration requirements of materials modelling.

Application of ontologies for materials science

Figure 7.9 illustrates the key aspects of the flow of data and knowledge from its generation, documentation, management and final exploitation as identified in the AMI2030 roadmap [11]. Ontologies play an important role for all these steps. Due to the limited scope, we will here only focus on data documentation and examples of industrial manufacturing cases using ontologies for data exploitation.

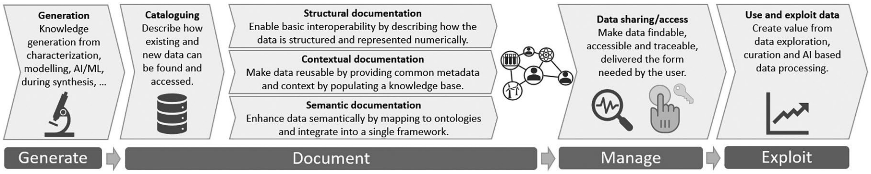

Figure 7.9 The flow of data from generation to exploitation and value creation. The labels at the bottom refer to the four priority topics in the AMI2030 roadmap, as illustrated in Figure 7.1. While cataloguing is an essential step for making data available for management and exploitation, is it possible to include or omit each of the three higher levels of data documentation.

Data documentation

Data documentation is the process of recording all relevant aspects of data to make it FAIR and facilitate its use and exploitation. Data can be documented at four distinct but interconnected levels:

Cataloguing provides a standardised way of describing and indexing data resources, making them easier for users to locate and utilise. It should provide sufficient information about where the data is located, the protocols used to access the data, the needed authentication and authorisation procedures, etc. to make it accessible. In addition, data catalogues also include standardised metadata, such as title, keywords, license, owner, project, contact person, format, etc., enabling a basic keyword-based search.

Structural data documentation describes how data is structured and represented numerically. It is an essential step for going from compatibility to interoperability. By standardising the description of the data representation, it becomes easier to combine and integrate data from various sources and make it more easily accessible to a broader range of users. The Datamodel Ontology [21] provides a standardised representation for data models that can help to ensure interoperability across different applications and contexts. This ontology is a simple yet comprehensive representation of the data, designed to be feature complete and easy to use. SFI Manufacturing has contributed to the development of DLite [22], which is a concrete implementation of an interoperability framework that uses the Datamodel Ontology.

Contextual data documentation is about providing sufficient context for the data to make it reusable. This is typically done by relating or linking the data items to other data items (aka *linked data*) in a knowledge base. For example, consider a dataset consisting of results from tensile tests from a series of welded joints between aluminium and steel. The obvious context that would be needed for most reuse of this dataset is the geometry of the welded sample, from where the sample is taken, how it is loaded, the composition and temper of the aluminium, steel and filler materials, type of welding and welding parameters such as temperature and welding speed. Additional useful context to this dataset would, e.g., be references to related datasets for the same sample, like TEM characterisation of the intermetallic phases that formed at different distances from the centre of the welding zone. Other metadata, like who performed the tests, when and in what project, is useful for search and data exploration. All such metadata can be expressed with RDF subject-predicate-object triples (each identified with an IRI)[1] in a knowledge base, resulting in a rich graph of linked data. In addition to reusability, contextual documentation also enables data exploration and semantic search.

Semantic data documentation expresses the shared meaning of the data by mapping it to concepts in published ontologies that are uniquely identified with IRIs. The logical structure of ontologies enhances the contextual data documentation by allowing the user to infer new relations between data items, as shown in the examples in Section "Application examples". Semantic data documentation enables the unambiguous exchange of knowledge and, thereby, cross-disciplinary and semantic interoperability. It also allows for advanced data exploration by exploiting the logical structure of the underlying ontologies.

Today, many data documentation systems only include cataloguing, limiting the use of their data to compatible systems, or requiring significant human intervention and effort to use their data. To increase the level of FAIRness and address the need for cross-disciplinarity and semantic interoperability, all levels of data documentation are required, supported by an ecosystem of ontologies and semantic tools.

Application examples

In this section, we will briefly describe two examples of how ontologies can be used for data exploitation in two real materials-related manufacturing cases originating from the OntoTrans [23] and OpenModel [24] EU projects.

Production of steel beam

Innovation: Energy-efficient, lightweight, and sustainable production of hot-rolled steel H-beams (Figure 7.10a), while meeting the demanding requirements on mechanical properties [25].

Challenge: To master the relationship between process parameters and the materials properties of the hot-rolled H-beams. Currently, process parameters and materials properties are managed via testing procedures, which use up significant time and resources and generate large sets of data.

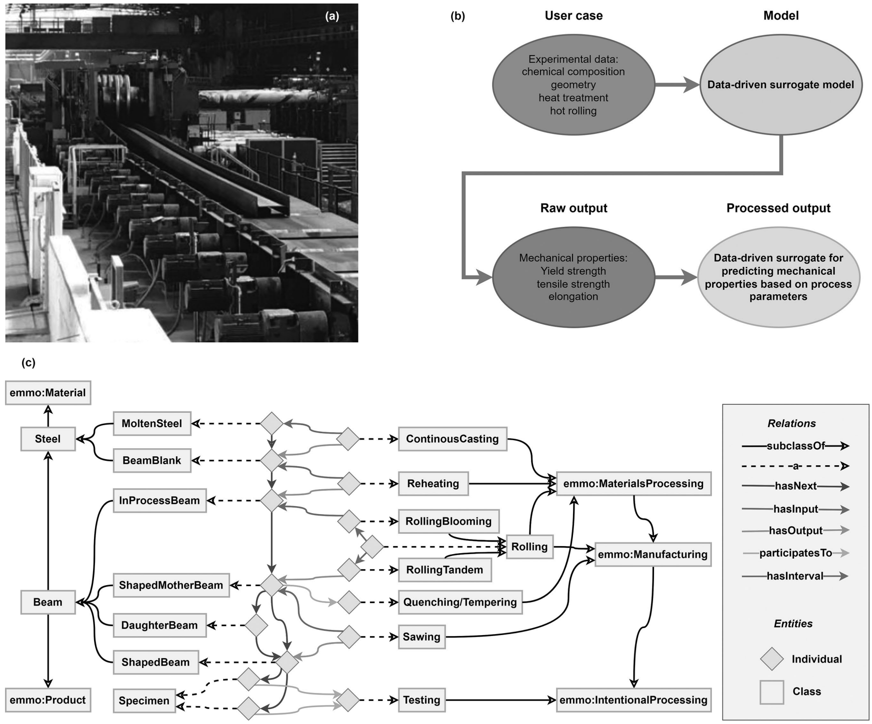

Figure 7.10 H-beams production line (a), modelling workflow (b) and semantic description (c)

Solution/Approach:

- Identify and define all the steps in the section mill steel beam manufacturing process (Figure 7.10b).
- Semantically document the case by ontologising the description of the underlying manufacturing processes (Figure 7.10c).
- Create data models for structural data documentation to exchange the data between the different tools.
- Create a surrogate model of the underlying system to allow efficient multi-objective optimisation (MOO).
- Perform MOO on the surrogate model to identify the Pareto optima cases, utilising the data models for interoperability.

Benefits semantic data documentation:

- More systematic description of the parameters and inter-relations.
- Connect the measured data to more generic concepts.

- The analysis is not dependent on the specific format provided by the plant; retrofitting or upgrading of the sensors or models is greatly facilitated.

Corrosion of aluminium-reinforced concrete

Innovation: Development of a new sustainable concrete mix tailored for aluminium reinforcement (less alkaline to avoid corrosion), with less energy intensive production, a significant reduction of CO_2 emissions, allowing slimmer lightweight concrete structures and a longer lifespan (leading to less waste) [26]. Figure 7.11a shows an aluminium-reinforced bench created for demonstration purposes.

Challenge: To predict and control the formation of the protective layer at the interface between the concrete and the aluminium reinforcement and to assess the resistance to corrosion under the load of the reinforced concrete. The analysis requires complex interactions between chemical reactions, aluminium microstructure, external loading, corrosion and the microlayer at the aluminium interface (Figure 7.11b).

Solution/Approach:

- Identify and define a modelling workflow to efficiently predict the protective layer behaviour (Figure 7.11c).
- Build an ontology to describe the material and the workflow (Figure 7.11d).
- Document the modelling tools, including their input and output, semantically.
- Utilise the OpenModel Open Innovation Platform to execute the workflow while optimising geometries and process parameters.

Benefits of semantic data documentation:

- Focus on the physics and concepts, abstracting away details about the underlying data format and representations.
- The semantic description of the models and workflow allows for model interchangeability (for example, replace Abaqus by Ansys).
- Facilitate the integration of experimental results for calibration and validation while relying on a common language.

Further perspectives

A standardised terminology will improve future exchanges among experts in the entire area of materials characterisation and modelling. It will facilitate the exchange with industrial end-users and researchers and reduce the barrier to utilise materials modelling. The common language is expected to foster dialogue and mutual understanding between industrial end-users,

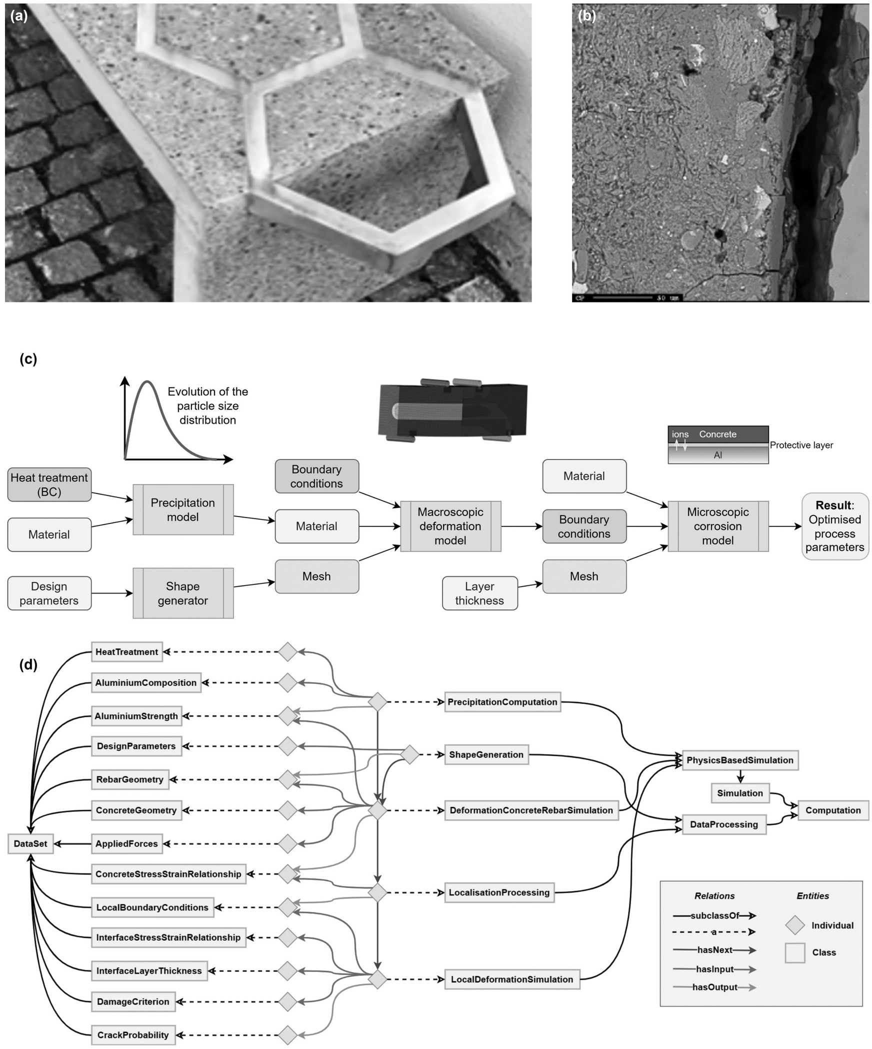

Figure 7.11 Aluminium-reinforced concrete and protective layer. (a) Demonstrator of an aluminium-reinforced concrete bench; (b) microstructure at the interface at the concrete-aluminium interface; (c) modelling workflow; (d) semantic description of the modelling workflow.

software developers, scientists, and theoreticians. It also constitutes the first step towards interoperability.

The development of EMMO is relevant for an integrated technological development and brings benefits for industrial end-users in terms of common understanding and improved communication, knowledge management, cross-discipline and semantic interoperability, consistent data interpretation and linking of resources, advanced search and data exploration, inferencing and reasoning and providing answers to queries that would otherwise remain unanswered. It will facilitate the digitalisation of materials and manufacturing and enable powerful AI applications.

We acknowledge the EMMC and AMI2030 initiatives as well as funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreements for OntoTrans (N^{o} 862136), OpenModel (N^{o} 953167) and OntoCommons (N^{o} 958371).

Note

1 Except for objects, which may also be a literal value.

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