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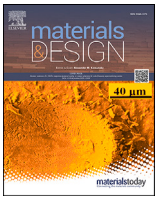

PMD Core Ontology: Achieving semantic interoperability in materials science

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ABSTRACT

Knowledge representation in the Materials Science and Engineering (MSE) domain is a vast and multi-faceted challenge: Overlap, ambiguity, and inconsistency in terminology are common. Invariant (consistent) and variant (context-specific) knowledge are difficult to align cross-domain. Generic top-level semantic terminology often is too abstract, while MSE domain terminology often is too specific. In this paper, an approach how to maintain a comprehensive MSE-centric terminology composing a mid-level ontology–the Platform MaterialDigital Core Ontology (PMDco)–via MSE community-based curation procedures is presented. The illustrated findings show how the PMDco bridges semantic gaps between high-level, MSE-specific, and other science domain semantics. Additionally, it demonstrates how the PMDco lowers development and integration thresholds. Moreover, the research highlights how to fuel it with real-world data sources ranging from manually conducted experiments and simulations with continuously automated industrial applications.

1. Introduction

The wide field of Materials Science and Engineering (MSE) is currently undergoing a dynamic digital transformation [1,2]. Several national initiatives aim to achieve an integral understanding of the entire materials life cycle, from raw materials to the operating components and beyond.[1],[2],[3],[4],[5] Automation, high-throughput methods, and data-based algorithms revolutionize production and characterization facilities.

It is of fundamental significance that material and process data, generated coherently in and by each step along entire value chains are comprehensively acquired, understandably processed, and shared in a controlled manner. If such data are continuously available at any point in the process chain, maximum efficiency of the entire cycle can be achieved. Seamless traceability could promote more innovative and environmentally friendly solutions in the various MSE branches. For example, raw materials could be better selected to incorporate more recycled materials. Moreover, if reliable material and process data were equally accessible, product lifetimes could be optimized by allowing for the precise tailoring of material properties and structures to specific application requirements [3].

The inherent diversity of MSE, encompassing perspectives from natural sciences such as physics, chemistry, and crystallography, along with methods from various engineering fields, presents a significant challenge to its digital transformation. Each discipline contributes its unique viewpoint, specialized terminology, and distinct data culture, which naturally leads to the presence of materials data in heterogeneous formats and structures.

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[1] https://www.plattform-i40.de/IP/Navigation/EN/.
[2] https://www.mgi.gov/.
[3] https://www.nims.go.jp/eng/news/press/2023/01/202301170.html.
[4] https://www.cnrs.fr/en/pepr/pepr-exploratoire-diademe-materiaux.
[5] https://materplat.org/en/.

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While these diverse data formats are a direct consequence of the inherent interdisciplinary nature of MSE, they further complicate communication within the MSE landscape. The variety in formats and structures, often incompatible with one another, hinders the seamless fusion of data, thereby impacting the exchange of information and knowledge [4]. This complexity hampers the automated acquisition, processing, and analysis of data and also impedes the advancement of data-driven approaches in material development [5,6].

In addition to the lack of uniform formats and structures, MSE data is frequently sparse or incomplete. Contextual information, including metadata and provenance, is often inadequately captured due to several reasons, such as the absence of proper experimental design information. As a result, processes, experiments, and simulations details are missing to represent them in a reproducible manner, limiting data reuse [7].

Addressing these challenges is vital for the successful long-term design of digital transformation in MSE, as this is expected to lead to improvements in existing value chains [8].

In this context, the MaterialDigital Initiative plays a pivotal role in addressing questions related to enhancing efficiency in the development of materials and products. It focuses on establishing the fundamental principles of digital methods and tools for MSE, addressing sustainability concerns, and applying them in an application-oriented manner [9]. Within this initiative, the Platform MaterialDigital (PMD)[6] provides support by developing prototype infrastructure and tool solutions for digital transformation, with the primary goal of assisting applied MSE with a focus on the industry.

Promoting semantic interoperability, which enables consistent data interpretation and exchange across platforms, in the broad field of MSE and among various drivers of digitalization is essential. This focus is evident at both national and international levels, particularly in initiatives such as Industry 4.0 and the National Research Data Infrastructure (NFDI).[7] The NFDI-Matwerk,[8] as part of this infrastructure, concentrates on the research field of MSE [10], underscoring the importance of a semantic interoperable approach. This approach fosters synergies and normalizes efforts across different domains, enabling the MSE field to benefit from data exchange in an agreed format that is distinct, shared, and well-defined. As digitalization encompasses more diverse systems, the need for a unified and scalable approach becomes increasingly vital, facilitating effortless access and utilization of information across various platforms.

To support information sharing and knowledge discovery, it is further recommended to adopt the Findable, Accessible, Interoperable, and Reusable (FAIR) principles, which outline the characteristics that modern data sources and infrastructures, tools, and vocabularies should possess [11,12]. In this context, the Semantic Web [13] offers existing technological capabilities and solutions for advanced data management, making its implementation highly beneficial for the MSE landscape [14].

To cope with the rapid progress of automation and the increasing volume of data, the creation and utilization of ontologies (ontology definition see [15]) are considered essential. This view is supported by recent discussions emphasizing the need for updated data management practices, including in particular the implementation of ontologies [16]. Ontologies are formal collections of concepts and their relationships, systematically and explicitly organizing knowledge in various domains, such as in the MSE domain [17], for both humans and machines, often employing a commonly agreed-upon, though not technically required, shared and consistent vocabulary. Ontologies reduce language barriers and ambiguities through standardized terminology, facilitating efficient data exchange and providing a clear mapping to the domain's context [18]. Future ontology-supported (meta)data acquisition, facilitated by software solutions such as laboratory information management systems (LIMS) and electronic lab notebooks (ELNs), promotes the establishment of complete and uniform data structures.

Ontologies facilitate the transformation of data into machine-understandable Resource Description Framework (RDF) triples, enabling seamless integration of materials data and promoting interoperable exchange [19–21]. This integration is further enhanced through the utilization of the SPARQL Protocol and RDF Query Language (SPARQL)[9] query language, which allows for automated and flexible retrieval of information from (meta)data triples stored in repositories, commonly referred to as triple stores. Moreover, reasoners[10] can derive valuable insights by analyzing the logical connections between ontological entities. While these technological tools contribute to efficient data handling and retrieval, it's important to note that the quality of data is determined by its original collection and curation processes. Access to high-quality data, critical for the progress of materials development, is thus dependent not only on these advanced technologies but also on the robustness of the underlying data generation and management practices [22].

Despite numerous efforts to develop ontologies for the MSE domain, many of them suffer from issues such as being unknown, inaccessible, poorly curated and maintained, and inadequately documented. Furthermore, these ontologies are often tailored for specific niches, lacking precise and domain-appropriate term definitions necessary for effective application and reuse [23,24].

Top-level ontologies (TLOs), such as the Basic Formal Ontology (BFO) [25] and the Descriptive Ontology for Linguistic and Cognitive Engineering (DOLCE) [26], are considered facilitators of cross-domain interoperability. Their high level of abstraction yields domain-independent, general concepts. However, the transition from domain-specific MSE application ontologies (AOs), which semantically represent specific processes, experiments, and simulations, to the abstract TLOs can be excessively complex.

To address this gap in MSE, we propose the PMD Core Ontology (PMDco) as a mid-level ontology aimed at promoting domain interoperability (see Fig. 1). Developed through continuous collaboration with the MSE community, the PMDco provides a selection of essential domain key terms within an intermediate semantic layer that is easily understandable and usable. It serves as an enhancer for future domain-specific AOs, facilitating connectivity to the PROV Ontology (PROV-O). PROV-O was developed by the World Wide Web Consortium (W3C) as a powerful tool for representing and exchanging provenance information across different systems and contexts [27]. Being on a higher domain-independent concept abstraction level, it is particularly useful in aligning observational data and models, providing a flexible model for process chain representations [28], and in mapping various ontologies [29]. Furthermore, the potential of PROV-O in identifying and relating entities and activities was shown in the generation of simulation models [30]. Therefore, PROV-O is a sound basis for MSE process and related materials data descriptions.

The PMDco supports the systematic creation of FAIR, high-quality materials data and plays an indispensable role in advancing semantic interoperability in MSE. Moreover, the PMDco holds significant potential in supporting international collaboration efforts, ensuring the consistent and efficient sharing of information and knowledge on materials. Further, by facilitating seamless data exchange and promoting a shared understanding, innovative and sustainable MSE research and development can be enabled.

In the following, a more detailed description of the requirements for the PMDco and its community-driven development process is being provided. In Section 3, the key specifications of the PMDco are presented, and its usage is explained through several examples. The sustainable im-

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[6] https://www.materialdigital.de/.

[7] https://www.nfdi.de.

[8] https://www.nfdi-matwerk.de.

[9] https://www.w3.org/TR/sparql11-query/.

[10] https://www.w3.org/2001/sw/wiki/Category:Reasoner.

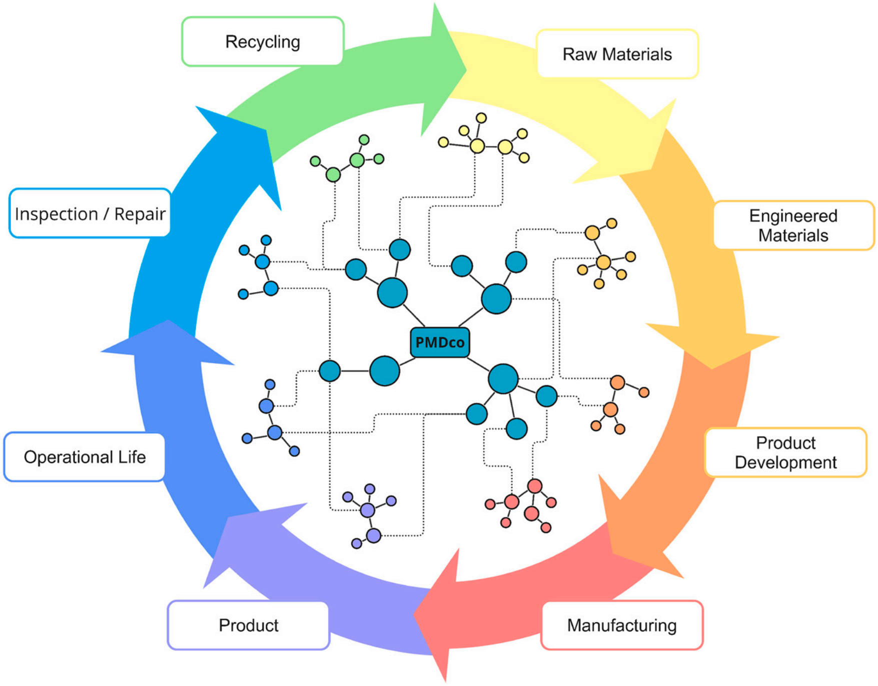

Fig. 1. Interoperable materials and process data. Relevant materials information across entire value chains is made consistently available through continuous process representations based on the Platform MaterialDigital Core Ontology (PMDco), enabling informed decision making at any given time.

plementation of maintenance and curation of the PMDco is described. In Section 4, the necessary actions and factors contributing to establishing the PMDco as an integral part of MSE knowledge representation are being discussed. Finally, in Section 5, this article is concluded with general remarks and an outlook for future work.

2. Ontology design and development

Key aspects and requirements that are of particular pertinence to the wide field of MSE and that strongly influence the design and development of the PMDco are presented below. It is further shown which connections to relevant ontologies are established.

2.1. Requirements for the PMDco

A primary goal of the digital transformation in the field of MSE is the comprehensive acquisition and transfer of materials information across the entire life cycle, ensuring its constant availability for retrieval and MSE knowledge extraction. As carriers of this information, (meta)data are generated at every step of the process chain and are represented via ontologies, enabling its subsequent (re)use.

Building on this, the MSE community aims to address additional aspects, according to the insights of a unpublished survey conducted among the 13 projects (involving MSE and ontology experts) funded in the first call of MaterialDigital. [31] Of particular interest to digitizers is the understanding of process-structure-property relationships, such as the profound influence of heat treatment parameters on the yield strength of steel materials. Another goal is the efficient transfer of prestructured data, such as in steel and copper keys, into knowledge graphs that provide novel query functionalities.

To meet these objectives, it is necessary to articulate specific requirements that will guide the development of the PMDco as a facilitator of domain interoperability. As such, the PMDco, positioned as a mid-level ontology for MSE, must encompass a broad spectrum of fundamental concepts within the field. This inclusivity empowers users to systematically formulate domain-specific ontologies describing their processes and link their process chains establishing semantic interoperability. Ensuring clear and unambiguous term definitions is essential for maintaining consistent and coherent representations of MSE knowledge that can be comprehended by both human and machine intelligence.

The PMDco should be publicly accessible and should also aim for optimal usability, which in this context refers to its ease of use and practicality. Eliminating barriers to entry, such as through detailed usage descriptions, provision of best practice examples, and interactive workshops, can facilitate adoption. A curation process involving the MSE scientific community will ensure the incorporation of necessary modifications and additions and turn it into a collaborative and community-supported endeavor. This collective effort is pivotal for fostering the healthy growth of the semantic foundation for MSE.

Diligent efforts should also be made to repurpose existing high-quality ontologies from related fields, such as chemistry. The use of the NeOn methodology is recommended in this context [32]. Aligning with established standards is crucial to enable seamless integration of data across diverse domains, thereby promoting knowledge exchange.

The utilization of the PMDco should enhance the reproducibility of processes and process chains, thereby catalyzing the systematic creation of rich FAIR datasets. Identifying recurring modeling patterns can progressively simplify query complexity, providing long-term benefits and optimizing the overall system.

2.2. Development process of PMDco

The PMDco development is based on collaborative efforts, involving continuous engagement with the MSE community, particularly the 20 PMD partner project consortia[11] from MaterialDigital funding phases 1 and 2. In developing the PMDco, our collaborative efforts concentrate on facilitating discussions, resolving modeling challenges, and gathering feedback from application ontology (AO) development and workshops. This approach is central to our methodology, which enables issues to be identified and solved together through constant exchange between ontology and domain experts. The goal is to iteratively evolve the PMDco and associated technologies to create a widely applicable

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[11] https://www.materialdigital.de/projects/.

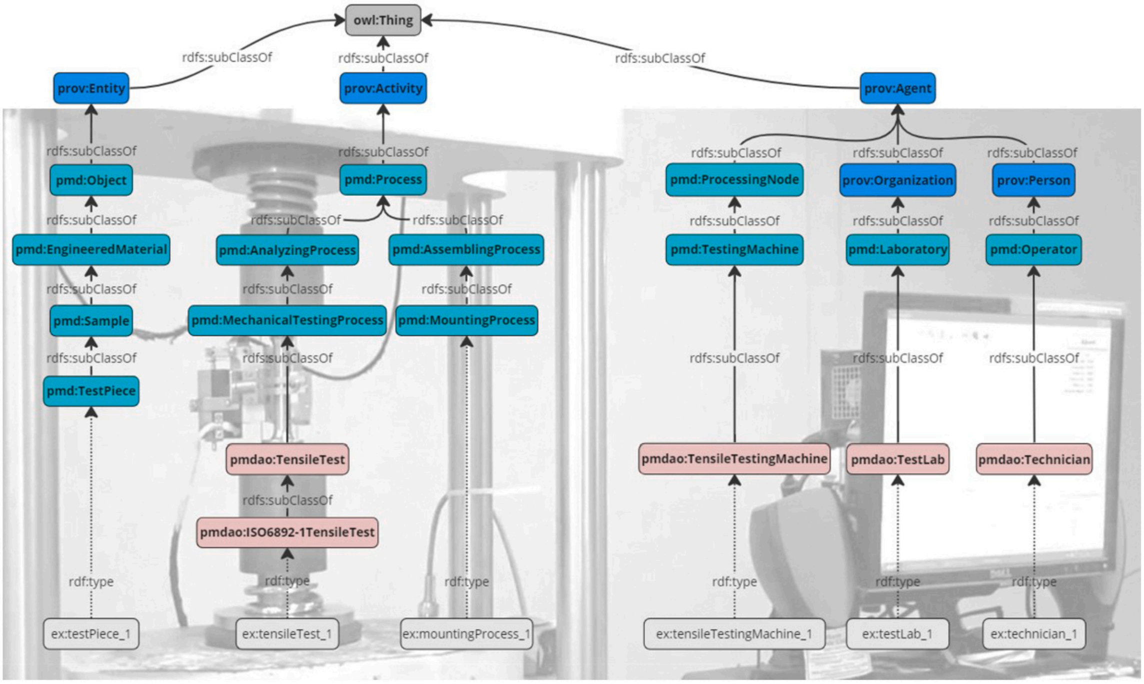

Fig. 2. Tensile test performed on a tensile testing machine and presentation of exemplary ontology components. Each class is a subclass of the top concept `owl:Thing`. Class connections are expressed via the property `rdfs:subClassOf`. PROV-O upper-level classes form the top layer. PMDco classes extend the class tree with MSE terms, providing necessary domain-specific semantics for connecting through tensile test vocabulary. Individuals are linked to the corresponding classes via the property `rdf:type`.

ontology framework for all MSE sub-domains. This process includes an interactive exchange using modeling examples to establish general-purpose representations. These representations are then incorporated into the PMDco documentation to facilitate usability. As a result of this effort, the PMDco 2.0.7 was recently published (see Section 3).

The PMDco development process utilizes various programming languages and tools. When working with MSE domain experts and ontology engineers in collaborative environments, tools that provide visualization capabilities for concepts and relationships play a significant role. These tools include Concept Board[12] and Miro.[13] OntoPanel is another graphical tool, based on a plug-in for the diagrams.net, designed to simplify ontology building for MSE domain experts [33].

The Protégé[14] ontology editor [34] was utilized to facilitate the design of semantically more expressive parts of the PMDco. Protégé is a widely used tool that supports the OWL 2 Web Ontology Language,[15] and it has the capability to run reasoners such as Pellet,[16] HermiT,[17] and FaCT++.[18] These reasoners help to reveal implicit information to users, enabling them to draw conclusions, make inferences, and identify inconsistencies, among other functionalities.

Python[19]-based libraries such as rdflib [35] and Owlready2 [36] are employed to facilitate semantic data processing within the PMDco and its associated AOs. The software development platform GitHub[20] is leveraged for publishing, continuous maintenance, and evolution of the PMDco through an implemented curation process. GitHub's integrated version control, bug tracking, and code review features are particularly beneficial in this regard. Additionally, GitHub houses the documentation for using the PMDco and its AOs.

2.3. PMDco basic layout aligned with PROV-O framework

The aforementioned key aspects, requirements, and ongoing engagement with the MSE community were considered in the selection of the PROV Ontology (PROV-O) framework for alignment of the PMDco (see Section 1).

As a mid-level extension of the PROV-O, the PMDco enables the representation and description of processes and process chains in a MSE-specific manner, ensuring full traceability of generated data points. Ontology-supported systematic information collection enables process reproducibility and increase quality in the long-term. The PMDco builds upon the three more abstract classes of the PROV-O, namely `prov:Activity`, `prov:Entity`, and `prov:Agent`, and enriches them using basic MSE terms. For example, it includes a direct subclass of `prov:Activity`, called `pmd:Process`, which serves as a superclass for more specific processes such as `pmd:AnalyzingProcess`, `pmd:AssemblingProcess`, and others (see Fig. 2). The PMDco comprises a vocabulary for describing PMDco (meta)data-generating processes, facilitating the development and integration of AOs. Specific AOs can extend the PMDco with additional terms and relationships. In future versions, these semantic boundaries can be redefined.

2.4. Reuse of other popular domain- and task ontologies

The PMDco follows an underspecified design on purpose being a versatile and extendable MSE mid-level. Valuable complementary ontological collections extend the expressive capabilities of the PMDco. For example, the Quantities, Units, Dimensions and Types (QUDT) [37] ontology collection can be used for expressing and converting units of measurement. Molecular entities such as atom, molecule, ion, ion pair, radical, radical ion, complex, conformer, etc. and chemical substances can be represented using the Chemical Entities of Biological Interest (ChEBI) [38].

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[12] https://conceptboard.com/.
[13] https://miro.com/.
[14] https://protege.stanford.edu/.
[15] https://www.w3.org/TR/owl2-overview/.
[16] https://github.com/stardog-union/pellet.
[17] http://www.hermit-reasoner.com/.
[18] https://fact-project.org/FACT++/.
[19] https://www.python.org/.
[20] https://github.com/.

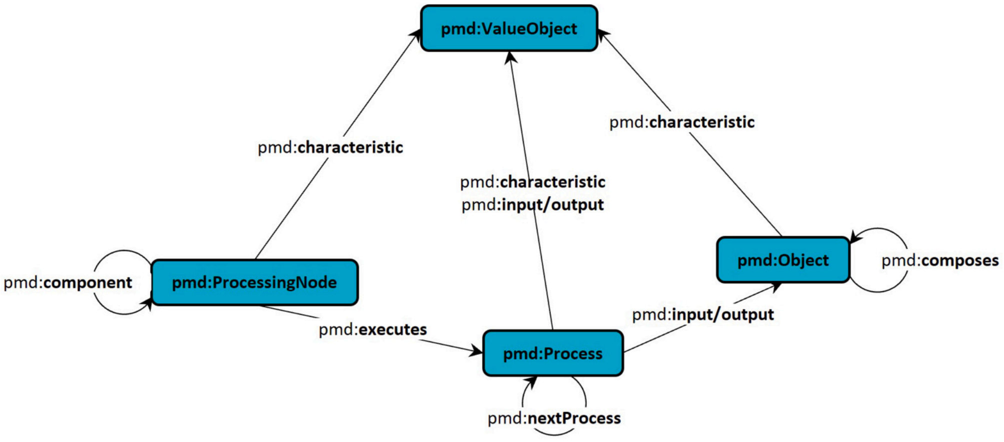

Fig. 3. The basic PMDco classes and their relations to each other. In the schematic arrangement, each `pmd:Process` is associated with `pmd:ProcessingNode` and `pmd:Object`. `pmd:ValueObject` is then allocated to these process-involved classes, serving as carrier for meta- and materials data. (For details on definitions of PMDco ontological entities, see https://w3id.org/pmd/co.)

3. The PMD core ontology

As a main contribution of this paper, details about the PMDco[21] are presented as results in this section. The PMDco satisfies the requirements presented in Section 2.1. Corresponding key features are summarized in the following.

3.1. Key features of the PMDco

- Comprehensive MSE vocabulary build on community consensus
  The PMDco offers a comprehensive MSE vocabulary developed through community consensus and in collaboration with MSE experts. It is highly comprehensible for domain experts and serves as a standardized foundation for representing MSE concepts and knowledge in a structured manner.
- Various mid-level classes to connect domain-specific AOs with top-level ontologies (TLOs)
  The PMDco incorporates mid-level classes that serve as connectors between domain-specific AOs and common TLOs. This linkage facilitates the integration of domain-specific knowledge with technical specifications, resulting in a more comprehensive representation of MSE processes and phenomena.
- Persistent unique identifiers for long-lasting referencability
  These identifiers, accessible at the PMDco namespace,[22] enhance the sustainability and interoperability of the knowledge representation by enabling reliable and persistent referencing and linking of concepts within the ontology.
- User-friendly, accessible and well-documented
  The PMDco prioritizes user-friendliness and accessibility with a well-documented open structure. The documentation, including step-by-step visual representations, serves as a valuable resource for researchers, practitioners, and developers working with materials data and applications. It offers a user-friendly approach for ontologically representing MSE (meta)data and knowledge using the PMDco.
- Core class layout is aligned with W3C PROV-O
  The PMDco class layout aligns with the PROV-O, enhancing its interoperability and potential reuse. This alignment ensures a clear, well-organized, and reliable foundation for the ontology.
- Reuse of other popular ontologies, such as QUDT or ChEBI
  The PMDco incorporates elements from popular task and domain ontologies like QUDT and ChEBI to leverage existing resources and promote interoperability. This reuse of ontologies establishes a bridge between different knowledge domains, expanding the applicability of the PMDco and facilitating the representation of interdisciplinary MSE concepts.
- Enabling reproduction of MSE processes and steps
  The PMDco enables the reproduction of MSE processes and materials properties by capturing relevant information and relationships. It supports the documentation and reconstruction of experiments, simulations, and other processes, enhancing transparency, reproducibility, and reliability in MSE research. This feature promotes scientific advancement and collaboration.

3.2. PMDco design

The PMDco is designed and applied based on its core classes: `pmd:Process`, `pmd:ProcessingNode`, `pmd:Object`, and `pmd:ValueObject` as well as their relations to each other (Fig. 3).

Processing nodes in the PMDco enable the execution of a process (step). They are semantically decoupled to be used for different types of processes, while the same process can be executed involving different nodes. Processing nodes are typically identifiable assets such as stationary experiment equipment, a steel mill, or a high performance simulation cluster. They are associated with processes via the `pmd:executes` property. Processing nodes may consist of additional components which is semantically implemented by using the `pmd:component` object property that relates processing nodes to other processing nodes or components (class `pmd:Component`). Analogously, objects can be composed of other objects using the `pmd:composes` property. Objects, such as engineered materials, blanks, samples, etc. are linked to processes as `pmd:input` or `pmd:output`. Multiple processes can be linked together via `pmd:nextProcess` and `pmd:previousProcess`. Processes can also be represented as hierarchies using the `pmd:subordinateProcess` property (see Section 3.2.4).

Processes, processing nodes and associated input and output objects are linked to specific characteristic (meta)data using the generic `pmd:ValueObject` class in the PMDco. Processes also require value objects to be an input or output. This design approach enables seamless and flexible traceability of meta- and materials data between processes and objects throughout value chains. It provides a solid semantic framework in support of the FAIR principles in MSE.

3.2.1. Process chain modeling

As indicated in the previous section, using the PMDco, enables the linking of several processes to form process chains (see Fig. 4). In this way, all contextual information required for data reproducibility can be included.

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[21] https://github.com/materialdigital/core-ontology.

[22] https://w3id.org/pmd/co/.

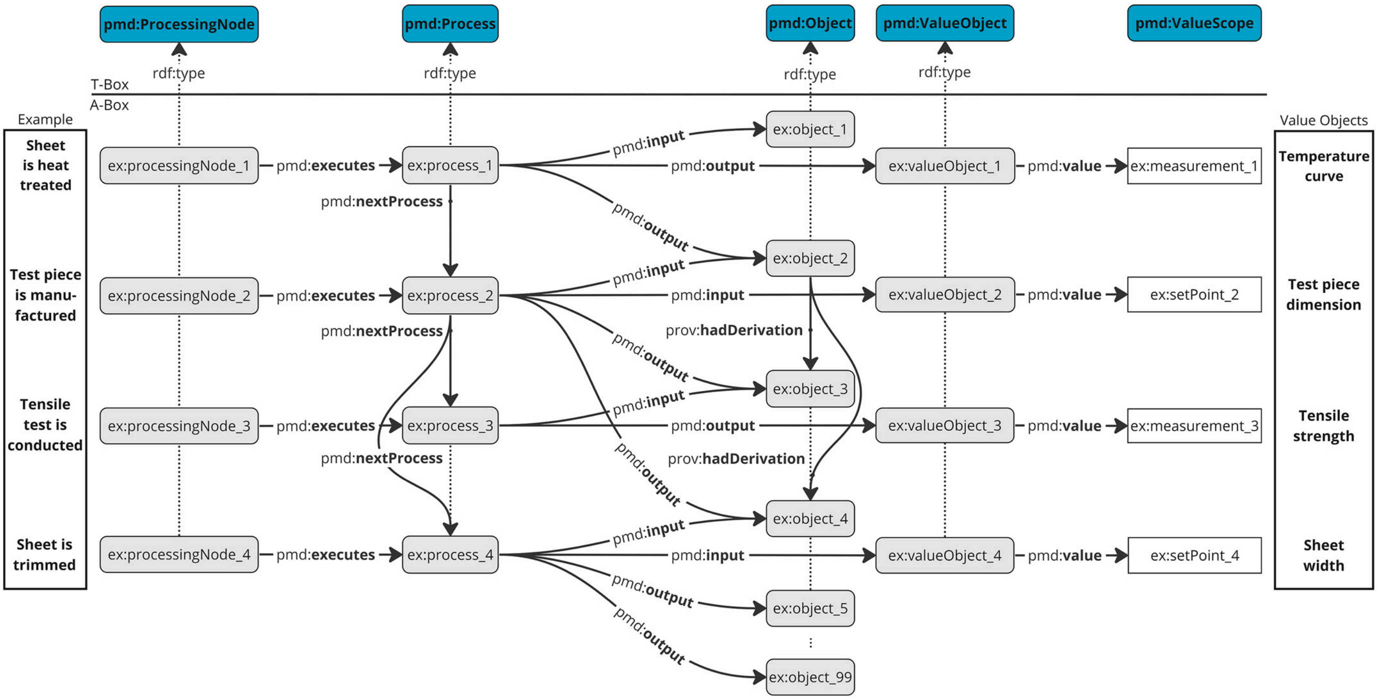

Fig. 4. Schematic representation of a typical MSE process chain: In this example, the T-Box is simplified to include basic classes of the PMDco for clarity. In the A-Box, the corresponding instances are linked to model a process chain: a steel sheet undergoes heat treatment. Subsequently, a tensile test is performed to determine the tensile strength of the heat-treated steel. If the mechanical properties improve, the sheet can be trimmed for further processing.

In the example shown a heat treatment process (process 1) is applied to a steel sheet (object 1) using a furnace (processingNode 1). The output of this process is the heat-treated steel sheet (object 2). The temperature curve (valueObject 1) is a measured output of this process (measurement 1). The next process in the sequence is the extraction of a test piece (object 3) for tensile testing. Object 3 and the slightly shortened heat-treated steel sheet (object 4) are derived from object 2. The required test part dimensions are specified as a set point input (setPoint 2) for the process. The tensile test (process 3) determines the tensile strength (valueObject 3) of the test piece (object 3) using a tensile testing machine (processingNode 3). In the final process (process 4), the shortened heat-treated steel sheet (object 4) is cut into pieces of equal width (object 5 - 99). The width (valueObject 4) is input for this process as a set point (setPoint 4).

PMDco users have the flexibility to choose the level of detail in their modeling. To provide further guidance for implementation, detailed excerpts based on the Fig. 4 are discussed below.

3.2.2. *Process and processing node modeling*

Fig. 5 demonstrates the modelling of a heat treatment process and its associated processing nodes. Processes execute processing nodes, which can be multi-component. The terminological box (T-Box) illustrates the subclass relationships, such as `pmd:HeatTreatmentProcess` being a subclass of the process, and `pmd:Furnace` and `pmd:Thermocouple` being subclasses of the processing node. The heat treatment temperature is the measured output of the process. In the assertional box (A-Box), the temperature value is provided in degrees Celsius, following the QUDT. Individual temperatures are categorized as a type of temperature, which is a subclass of both the value object and the value scopeś measurement subclass. Processing nodes can also have metadata directly assigned to them, as seen in the example with the depiction of the thermocoupleś node series. Further details on value and data scope modelling can be found in Section 3.2.5.

3.2.3. *Process and object modeling*

Processes have objects as input and output. In Fig. 6, a manufacturing process is illustrated where a heat-treated sheet is used as the input. During the process, a part of the sheet is cut off to produce a tensile test piece. Consequently, the output includes both the test piece and the shortened heat-treated sheet. These two output objects have their origin in the heat-treated sheet, which is expressed with `prov:hadDerivation`. To provide additional information, objects can be assigned characteristic metadata. For example, the test piece is given a string name value “TT42aaa”, categorized as an identifier and a value object. The original thickness of the test piece serves as a input set point for the manufacturing process and is represented as a new class, also typified as primary data for enhanced differentiability. The value of the original thickness is specified in millimeters using the QUDT unit, utilizing a float data type.

3.2.4. *Process sequence modeling*

The PMDco design allows for the effective modelling of processes as sequences using properties like `pmd:nextProcess` and `pmd:previousProcess`. Additionally, to further partition individual processes, properties such as `pmd:subordinateProcess` and `pmd:superordinateProcess` can be leveraged. Time information, such as start and end times, can be captured using the `xsd:dateTime` datatype. In Fig. 7, an example of a process chain is depicted, involving a measuring process, a two-step assembly process, and a mechanical testing process. This modelling approach can accommodate arbitrarily complex process chains while also allowing for a less detailed representation.

3.2.5. *Value scope and data scope modeling*

In the PMDco, value objects play a crucial role in representing specific values associated with processes, processing nodes, and objects. The `pmd:characteristic` and `pmd:input/output` properties are used to establish these associations (as shown in Fig. 3). Value ob-

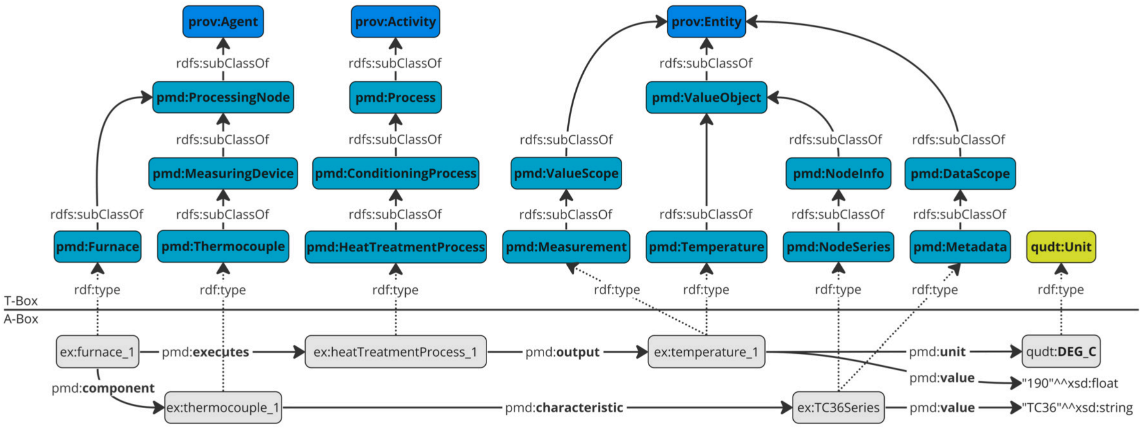

Fig. 5. Process and processing node modeling. A furnace executes a heat treatment process. The thermocouple serves as a component of the furnace. Metadata can be specified to provide information about processing nodes, such as the series of the thermocouple. The temperature measurement is output of the heat treatment process.

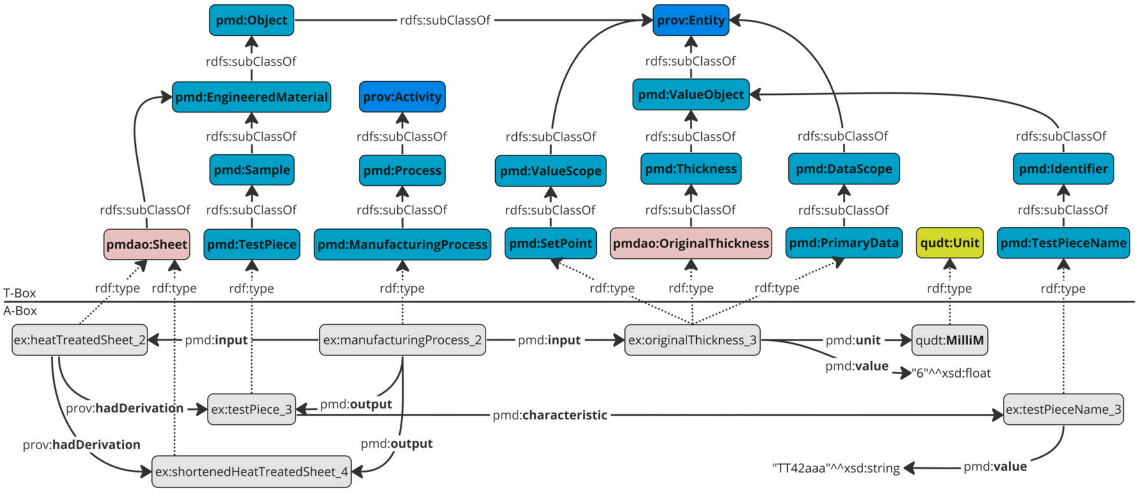

Fig. 6. Processes have objects as input and output. A manufacturing process is depicted as having a heat-treated sheet as input. During this process, a portion of the sheet is cut off to create a test piece for a tensile test. The shortened sheet is also produced as an output of the process. Metadata, such as the name of the test piece, can be specified to provide additional information about the objects involved. The required dimensions of the test piece are linked to the process as a set point.

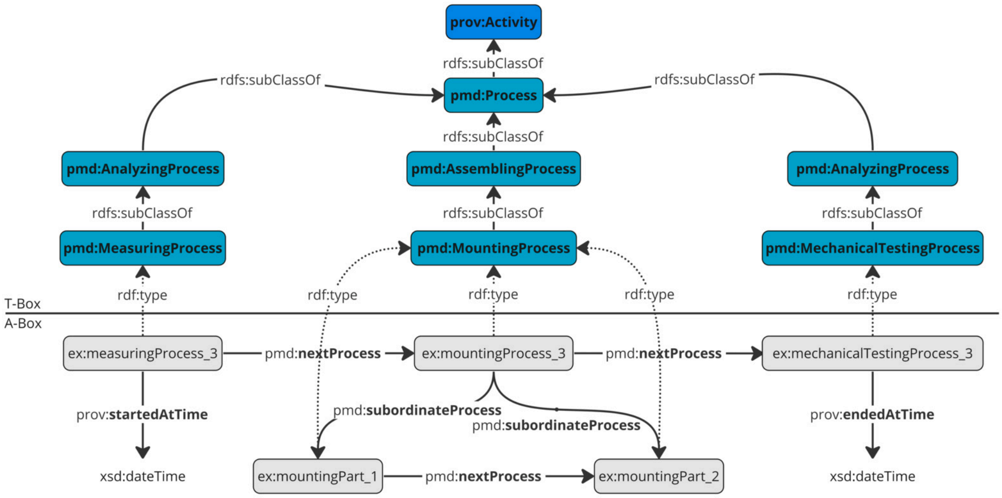

Fig. 7. Process sequences and process chain modeling. Processes in the PMDco can be linked to subsequent processes using the concept of next process. In the given example, the measurement process is followed by a mounting process, which in turn precedes the mechanical testing process. Furthermore, the mounting process consists of two subordinate processes.

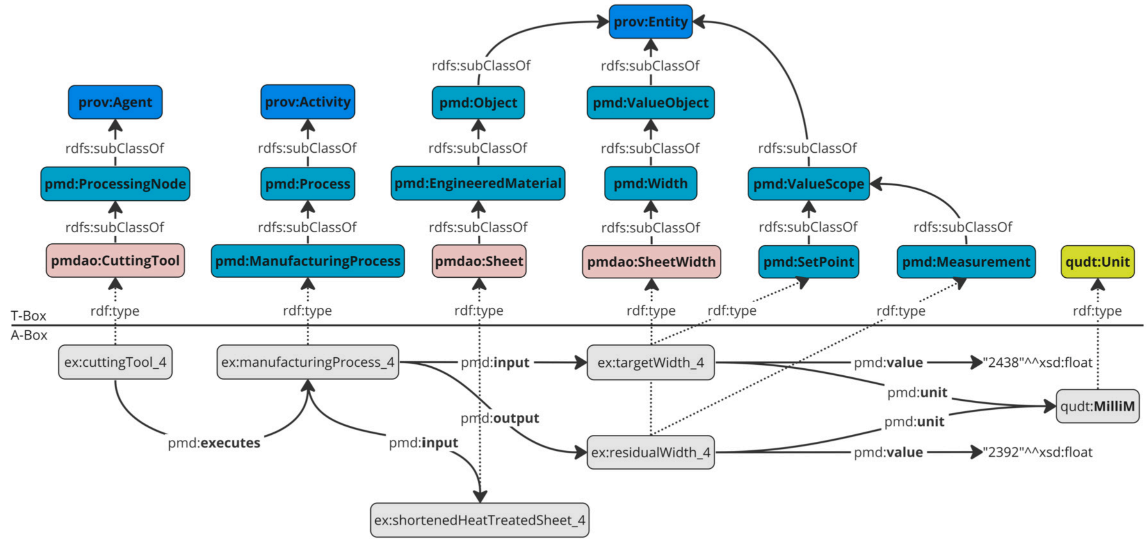

Fig. 8. Value scope modeling. In this figure, the concept of differentiating value objects into measurement and set point subclasses of `pmd:ValueScope` is depicted. The manufacturing process involves cutting a sheet into equal pieces with a specified width of 2438 mm, identified as a set point. However, it is observed that the last piece of the sheet, when measured, has a width of only 2391 mm, making it unsuitable for use.

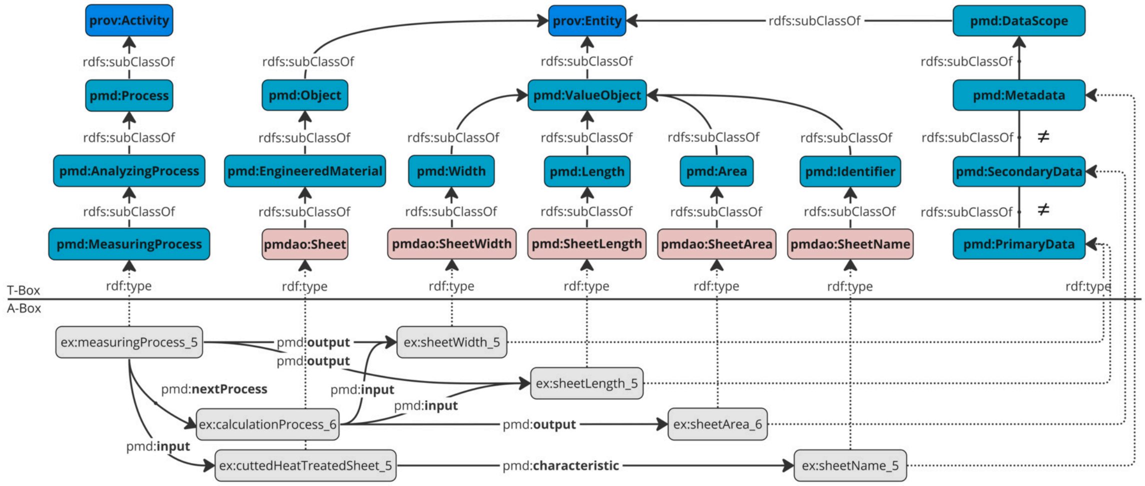

Fig. 9. Data scope modeling. The assignment to the `pmd:DataScope` subclasses allows for differentiation between primary, secondary and metadata. In a measurement process, the sheet width and sheet length are measured as primary data. The sheet area is then calculated from these input measurements, resulting in secondary data. Additionally, the identifier of the sheet is considered metadata.

jects can represent various types of values, including numeric, textual, and complex data structures. Literal values are represented using the `pmd:value` data type property. Units from the QUDT ontology can be linked to value objects using the `pmd:unit` property. The `pmd:resource` property allows for linking value objects to URIs.

To ensure proper differentiation of value objects, the ontology introduces value scope subclasses, including `pmd:Measurement` and `pmd:SetPoint` (see Fig. 8). This classification gains particular significance when processes are constrained to specific input set points. The measurement subclass indicates that the value objects have been measured or determined, enabling correlations and relationship establishment.

The PMDco also provides data scope subclasses, including `pmd:Metadata`, `pmd:PrimaryData`, and `pmd:SecondaryData`, for further classification of value objects (shown in Fig. 9). Metadata include contextual information, as well as provenance details, which are essential for a comprehensive understanding of processes and steps. Primary data or raw data are acquired directly by a process, experiment or simulation. Secondary data can subsequently be deduced from these.

3.3. *Reuse of existing ontologies*

Reusing existing ontologies is an important practice in the development of the PMDco. By bridging semantic gaps and identifying equivalent or related concepts across different ontologies, meaningful communication and collaboration can be facilitated among disparate data sources. This allows for enhanced data interoperability, knowledge sharing, and a more comprehensive domain understanding. Reusing well-defined concepts from established ontologies saves time and effort and promotes consistency, standardization, and knowledge accumulation within a broader community [39,40].

The PMDco incorporates concepts from well-known ontologies to enhance its functionality and interoperability. The QUDT, as a well-engineered and comprehensive ontology and vocabulary, is used to express physical and mathematical units in the field of MSE, including metric prefixes. It provides a unified model for quantities, dimensions, units, and instances data. The conversion functionality between single and complex types of units can be considered particularly useful.

The ChEBI ontology is utilized for the ontological representation of chemical entities, providing a comprehensive dictionary and ontology for small molecular entities. It describes various types of atoms, molecules, ions, radicals, and more. Furthermore, ChEBI incorporates an ontology, in which relationships between compounds, groups or classes of compounds and their parents, children and siblings are specified. Therefore, it is predestined for reuse in terms of referring to chemical entities, especially using the chemical entity class `obo:CHEBI_24431`.[23] In this way, chemical compositions, which represent an important material property, can be described. The linkage with entities of the ChEBI establishes important cross-domain connections.

The Character-Separated Values on the Web (CSVW)[24] standard is used to describe primary data originally available in Character-Separated Values (CSV) format, which is commonly used in MSE measurements. It clarifies the content of CSV tables, including the file source (`csvw:url`), schema (`csvw:schema`), and metadata information (e.g., `csvw:name`, `csvw:datatype`).[25]

The DataCite[26] ontology enables the description of metadata properties for resource identification and citation purposes (e.g., `datacite:Identifier`),[27] aligning with the DataCite Metadata Scheme Specification.

3.4. Maintenance and curation

The PMDco is continuously updated and maintained through ongoing interaction with the MSE community. A vital building block in support of community interaction is the Ontology Playground. The Ontology Playground[28] functions as a collaborative space that is an open forum for discussion and feedback from experts in the field. It is usually attended by around 20 participants from the MSE community, including all participant projects. The insights gained from this forum form an important basis for the PMDco curation process. The curation process is carried out using GitHub functionalities and is an essential part of active participation in the development of the PMDco. This involves updating terms and definitions, adding new concepts, and removing obsolete ones. To ensure quality and usefulness, the ontology is continuously curated through structural improvements and the identification of gaps and inconsistencies. To manage ontology maintenance effectively, the following aspects and considerations should be implemented:

- Version control: GitHub is used as a version control system to track and manage changes, allowing for easy comparison and reversion to previous versions if needed.
- Documentation: Thorough documentation is provided, including the PMDcoś purpose, scope, design decisions, and any known limitations. Guidelines for usage and contribution are also provided to help users and maintainers understand the ontology and its updates.
- User feedback: Active solicitation and encouragement of user feedback play a crucial role in identifying errors, ambiguities, or missing information. The GitHub environment serves as a platform for users to report issues and suggest improvements.
- Quality assurance: Quality checks are performed at regular intervals to ensure accuracy, consistency, and compliance with design principles. Automated reasoning tools and validation scripts are utilized to detect logical inconsistencies or violations of predefined constraints.
- Community engagement: Encouraged through events like the biweekly Ontology Playground, this interactive forum promotes collaboration and feedback among domain experts and stakeholders from all consortia within the Platform MaterialDigital (PMD). Within this publicly accessible exchange forum, participants share modeling challenges, propose solutions, and discuss the development of complementary tools.
- Continuous updates: The PMDco is regularly updated by incorporating new knowledge, domain advancements, and user feedback. Staying informed about relevant research, publications, and data sources helps identify necessary changes or additions to the ontology.
- Evolving requirements: Alignment with changing user requirements and contexts is evaluated. Ensuring the ontology remains relevant and adaptable to new use cases and emerging technologies is a priority.
- Collaboration and coordination: Effective mechanisms are established within the PMDco maintenance team. Clear roles and responsibilities, communication channels, and collaboration tools are used for efficient teamwork.

During the development of the PMDco, all but one of the aspects illustrated above were implemented. The only exception that is still work in progress is the aspect of quality assurance. The definition of appropriate and automatable quality checks requires a large volume of instantiated named individuals in knowledge graphs. While being complete and consistent on a case-to-case basis, the quantity of available real-world use cases the PMDco is based on did not reach the critical mass required to evaluate the feasibility and applicability of corresponding quality checks.

In general, implementing these strategies ensures the ongoing integrity, usefulness, and quality of the PMDco for the MSE community.

4. Discussion

4.1. Continuous, community-driven advancement

The PMDco is continuously being engineered to enable detailed modeling of process chain(s) and constituent processes, so that materials data can be comprehensively acquired and shared across entire value chains. To achieve this, the PMDco provides an appropriate mid-level framework for the MSE domain. Its easy-to-use and generic MSE vocabulary and comprehensive documentation support the usage and creation of domain-specific AOs. These AOs connect and enrich the provided mid-level concepts, with specific MSE vocabulary relevant to their use cases. As a demonstration of this process, a standards-compliant AO[29] was designed to represent the tensile test of metals at room temperature as defined in ISO 6892-1:2019-11 [41], serving the purpose of providing consistent and FAIR structures for tensile test data.

Further aspects have to be considered for positioning the PMDco as a robust and widely accepted framework for the generation of FAIR data structures and further, as one of the enablers for digital transformation in MSE in the long run.

The curation and maintenance process outlined in Section 3.4 requires close monitoring and scalable implementation in progressive exploitation. Similar to other ontologies, the PMDco is subject to continuous improvement and refinement to reflect the latest advances and modifications in the domain. Thus, active engagement with the community is essential for establishing the PMDco as a valuable and actionable standard for the MSE domain. Vital interaction with users and interested stakeholders is facilitated through the aforementioned Ontology Playground. The establishment and sustainability of the GitHub-based curation process make it feasible for individuals to actively contribute to shaping the PMDco.

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[23] ChEBI namespace: http://purl.obolibrary.org/obo.

[24] https://csvw.org/.

[25] CSVW namespace: http://www.w3.org/ns/csvw#.

[26] http://www.sparontologies.net/ontologies/datacite.

[27] DataCite namespace: http://purl.org/spar/datacite.

[28] https://forum.materialdigital.de/t/onboarding-semantische-interoperabilitaet.

[29] https://github.com/materialdigital/application-ontologies/tree/main/tensile_test_ontology_TTO.

4.2. Enrichment and interoperability

With the goal of expanding PMDcoś range of applications, it is essential to evaluate and incorporate existing works into future versions. For instance, integrating detailed material structure information can significantly enhance PMDcoś versatility by enabling more precise material characterization and analysis. A comprehensive collection of microstructure descriptors is available in the reference [42]. Beyond, the Elementary Multiperspective Material Ontology (EMMO)[30] offers valuable insights for modelling distinct physical materials. Establishing mappings and alignments with existing ontologies, as well as reuse of concepts of other ontologies, are important practices that can further facilitate seamless interactions and data exchange between ontologies [43–45].

Beyond domain boundaries, mappings to BFO top-level concepts become desirable for achieving cross-domain interoperability. Although there are different proposals for mapping the PROV-O to the BFO, a definite solution is yet to be established [28,46,47]. The mapping of `prov:Activity` to `bfo:Occurent` and `prov:Entity` to `bfo:Continuant` has emerged as the most promising option. Further alignment with the BFO will be addressed in future PMDco versions.

4.3. International collaborations

Active participation in significant work and interest groups will be particularly supportive for interdisciplinary exchange and future collaborations. The PMDco's involvement and positioning in the newly founded MSE working group, of the Industrial Ontologies Foundry (IOF),[31] is particularly valuable in terms of realizing data interoperability in the entire field of digital manufacturing in the industrial domain. Similarly, contributions to the Materials Data, Infrastructure and Interoperability IG[32] and MaRDA[33] working groups, of the Research Data Alliance (RDA),[34] form cornerstones of international collaborations and exchange of knowledge between standardization bodies, from which new insights and definitions of common MSE data standards are emerging.

4.4. Incentives and amplification effects

An amplifier for the discoverability and reusability of the PMDco and related AOs, ontology repositories such as MatPortal[35] or the terminology service of NFDI4Ing[36] are playing a crucial role. Automated mechanisms of ontology sharing across different projects and domains could be established for reducing development efforts. Repositories foster harmonized growth of ontological knowledge by providing various capabilities, such as identification of ontological entities, and consequently facilitating AO developments. Further incentives can be created by integrating the PMDco and its AOs with already established tools in use. ELNs enable the linking of input fields to ontological entities. Through a script, the inputs are then directly transformed into RDF triples. The compiled ELN templates are easily distributed and utilized, and as a consequence facilitate low-threshold technological implementation for the creation of uniform, FAIR data structures with improved process and experiment reproducibility. Obviously, in the future, more video tutorials and best practice examples have to be produced and published. The same applies to on-going interactive workshops for using the PMDco.

5. Conclusion

In conclusion, the PMD Core Ontology (PMDco) represents a significant advancement in the digital transformation of Materials Science and Engineering (MSE). MSE, being a multidisciplinary field, faces challenges in effectively exchanging information and knowledge due to diverse perspectives, specialized terminology, and incompatible data formats. These hurdles impede the seamless fusion of (meta)data and hinder progress in data-driven approaches in materials development.

To overcome these challenges, the PMDco serves as robust mid-level ontology that promotes domain interoperability in MSE. It provides a shared and consistent vocabulary, enabling the transformation of process and materials data into machine-processable RDF triples, facilitating their integration and exchange following FAIR principles. The PMDco supports the creation of high-quality data structures, enhancing reproducibility and reusability of MSE processes, experiments, and simulations as well as materials data.

One baseline contribution of the PMDco is its pivotal role in enhancing semantic interoperability. It bridges the semantic gap between domain-specific MSE ontologies and upper-level ontologies as well as domain-independent modules, such as the PROV-O, facilitating cross-domain connections. The PMDco establishes a stable intermediate semantic layer that is easily understandable and usable, promoting efficient exchange of (meta)data and a shared understanding among MSE researchers and practitioners.

To ensure the usability and evolution of the PMDco, a transparent and community-driven curation process on GitHub enables active participation from the MSE community in advancing the PMDco. This process, akin to other community-driven processes such as paper reviews or the collaborative refinement in Wikipedia curation, needs to establish itself within the community to function effectively. By connecting AOs and incorporating domain-specific terms and concepts, the PMDco expands and enriches itself, accommodating the diverse aspects of MSE.

The development of a standard-compliant AO for the tensile test of metals at room temperature, following ISO 6892-1:2019-11 [41], exemplifies how the PMDco can be utilized in AO development. This demonstrates the practical usage of the PMDco and its extension to domain-specific terms and concepts across other AOs within the PMD project and beyond.

To ensure ongoing maintenance and sustainability of the PMDco, a committee of MSE and ontology experts will need to review proposed changes. This collaborative approach encourages community involvement and supports the continuous evolution of the PMDco. Furthermore, collaborative work on ontologies within the MSE community is inclined to lead to the emergence of advanced tools that facilitate ontology development and data mapping processes, benefiting the scientific community as a whole, as can be seen in recent tool developments in connection with digitalization initiatives such as OntoPanel [33] and Fast OntoDocker.[37]

Looking ahead, the success of the PMDco relies on the active involvement from the MSE community. Integrating AOs enables the PMDco to capture a broader range of MSE knowledge and expand its capabilities. The curation process on GitHub allows experts to contribute, ensuring transparency, version control, and community engagement. Collaborations with ongoing PMD partner projects and other communities offer opportunities for further research and improvements, such as integrating the PMDco with EMMO ontology mappings.

In summary, the PMDco represents a significant milestone in advancing semantic interoperability and knowledge sharing in MSE. By providing a common vocabulary, supporting FAIR data principles, and promoting collaboration, the PMDco serves as a valuable resource for researchers and practitioners, enabling scientific discovery and inno-

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[30] https://github.com/emmo-repo/EMMO.

[31] https://www.industrialontologies.org/.

[32] https://www.rd-alliance.org/node/939.

[33] https://www.marda-alliance.org/.

[34] https://www.rd-alliance.org/.

[35] https://matportal.org/.

[36] https://terminology.nfdi4ing.de/ts/.

[37] https://github.com/materialdigital/ontodocker.

vation in MSE and related domains. Through continuous community collaboration, ongoing maintenance, and the catalyzed integration of AOs, the ontological framework of the PMDco will continue to evolve and contribute to the digital transformation of MSE, fostering advancements in materials development and facilitating sustainable research and development practices.

A-Box	assertional box
AO	application ontology
AOs	application ontologies
BFO	Basic Formal Ontology
CSV	Character-Separated Values
ChEBI	Chemical Entities of Biological Interest
CSVW	Character-Separated Values on the Web
DOLCE	Descriptive Ontology for Linguistic and Cognitive Engineering
EMMO	Elementary Multiperspective Material Ontology
FAIR	Findable, Accessible, Interoperable, and Reusable
MSE	Materials Science and Engineering
PMD	Platform MaterialDigital
PMDco	Platform MaterialDigital Core Ontology
PROV-O	PROV Ontology
QUDT	Quantities, Units, Dimensions and Types
RDF	Resource Description Framework
SPARQL	SPARQL Protocol and RDF Query Language
T-Box	terminological box
TLOs	top-level ontologies
W3C	World Wide Web Consortium

Prefixes of ontologies and vocabularies mentioned:

`bfo:` http://purl.obolibrary.org/obo/
`chebi:` http://purl.obolibrary.org/obo/CHEBI_
`csvw:` http://www.w3.org/ns/csvw#
`datacite:` http://purl.org/spar/datacite/
`ex:` https://example.org/
`pmd:` https://w3id.org/pmd/co/
`pmdao:` https://w3id.org/pmd/ao/
`owl:` http://www.w3.org/2002/07/owl#
`prov:` http://www.w3.org/ns/prov#
`rdf:` http://www.w3.org/1999/02/22-rdf-syntax-ns#
`rdfs:` http://www.w3.org/2000/01/rdf-schema#
`qudt:` http://qudt.org/schema/qudt/

CRediT authorship contribution statement

Bernd Bayerlein: Writing – review & editing, Writing – original draft, Visualization, Supervision, Software, Methodology, Investigation, Conceptualization. **Markus Schilling:** Writing – review & editing, Writing – original draft, Software, Methodology, Investigation. **Henk Birkholz:** Writing – review & editing, Writing – original draft, Conceptualization. **Matthias Jung:** Writing – review & editing, Methodology. **Jörg Waitelonis:** Writing – review & editing, Supervision, Software, Methodology, Investigation, Conceptualization. **Lutz Mädler:** Writing – review & editing, Funding acquisition, Conceptualization. **Harald Sack:** Writing – review & editing, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The PMD Core Ontology can be readily obtained by downloading it from the following repository [https://github.com/materialdigital/core-ontology].

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Appendix A. Supplementary material

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