

Semantic modelling of Process-Structure-Property dependencies of rolled metal sheets

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Abstract

Unraveling process-structure-property (PSP) dependencies in materials science and engineering remains a significant challenge due to the highly complex interdependencies, heterogeneity and incompatibility of data across various sources. Ontology-based knowledge representation offers a framework for the formal, machine-actionable description of such dependencies, supporting FAIR data principles and logical reasoning. PSP dependencies are particularly complex for rolled metal sheets, whose manufacturing process chain determines the resulting microstructure and crystallographic texture. The latter governs the anisotropy of functional properties, which is critical for material selection and performance optimization. In this work, semantic models are presented for describing PSP dependencies in rolled metal sheets, covering the manufacturing process chain, microstructural features, crystallographic texture, and the anisotropy of functional properties. The models are aligned with the Basic Formal Ontology (BFO) via the Platform MaterialDigital Core Ontology (PMDco 3.0), ensuring semantic interoperability. The framework is validated for the use case of non-oriented electrical steels (NOES), an essential material for electromobility, to demonstrate the applicability of the proposed models to an industrial domain. The presented semantic models enable systematic data integration and knowledge reuse, and provide a foundation for graph-based, data-driven approaches for multi-objective materials optimization.

Keywords

semantic modeling, ontology engineering, process-structure-property dependencies, rolled metal sheets, crystallographic texture

Introduction

Rolled metal sheets are structural and functional materials widely utilized in electrical engineering, automotive engineering, and construction¹. Their performance is governed by complex process-structure-property (PSP) dependencies, as illustrated in Figure 1. Chemical composition and manufacturing process chain, including sequential rolling passes and heat treatments, determine the resulting microstructure and crystallographic texture. Microstructural features, such as average grain size and the presence of inclusions and precipitates, affect functional properties of finished metal sheets in opposing ways. For instance, in soft magnetic metal sheets, grain growth reduces core losses but decreases strength^{2,3}. Crystallographic texture, which develops during rolling, governs the anisotropy of functional properties within the rolling plane (RP)^{4,5}. The resulting property anisotropy poses challenges for material selection and component design for a given application. The explicit correlations of PSP dependencies enable inverse material design, in which the manufacturing process chain and the choice of alloying elements are optimized to achieve target functional properties^{3,6,7}.

To address the high dimensionality and complexity of the PSP dependencies, data-driven approaches have been widely applied in the MSE domain^{8–10}. However, the effectiveness of such methods depends on the availability of high-quality structured data^{11,12}. Data integration remains

a bottleneck for data-driven methods in MSE, as the data is often incomplete, provided in heterogeneous formats, and incompatible across different sources. The challenge can be mitigated by adopting Findable, Accessible, Interoperable, and Reusable (FAIR)¹³ data principles in the MSE domain, enabling machine-actionable and reusable representation of domain knowledge. Ontologies, formalized using the W3C Web Ontology Language (OWL 2)¹⁴, provide a semantic framework for the formal description of the domain of interest and support alignment with the FAIR data principles^{15–17}. Furthermore, OWL 2 supports logical reasoning over data in the knowledge graph (KG) format, allowing inference of implicit domain knowledge beyond explicitly asserted facts, which is particularly valuable for understanding complex PSP dependencies of rolled metal sheets. In the MSE community, ontology-based approaches have been widely adopted within the

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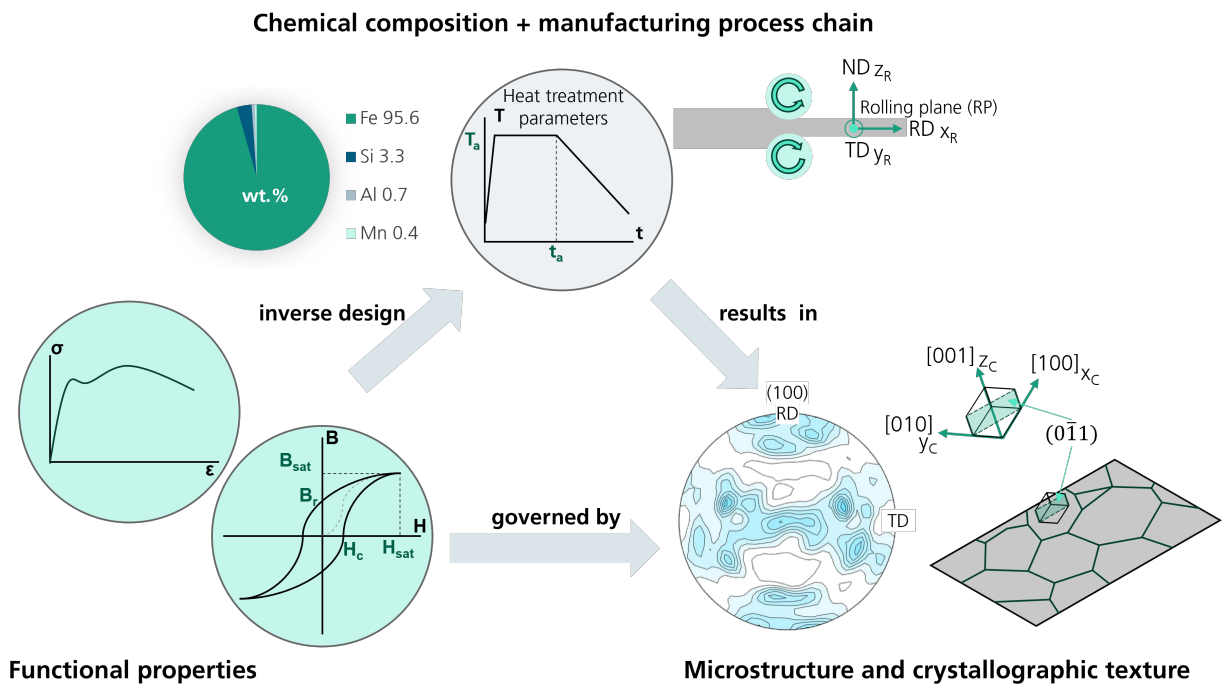


Figure 1. Overview of PSP dependencies of rolled metal sheets. The chemical composition and manufacturing process chain determine the microstructure and crystallographic texture of the finished rolled sheet. The crystallographic texture is characterized by the preferred grain orientation, expressed as a relation between the crystal reference frame (x_C, y_C, z_C) and the rolling reference frame (x_R, y_R, z_R) defined by the rolling, transverse, and normal directions (RD, TD, and ND, respectively). Functional properties are represented by a stress-strain curve (mechanical) and a hysteresis loop (magnetic), both governed by the microstructure and exhibiting anisotropy due to preferred grain orientations. The inverse design arrow indicates that explicit knowledge of PSP dependencies enables targeted optimization of composition and process chain to achieve desired material properties.

European Materials Modelling Council (EMMC)¹⁸ and the Platform MaterialDigital (PMD) initiative¹⁹, demonstrating the viability of semantic data representation across heterogeneous MSE datasets.

In the present work, semantic models are introduced to formally describe PSP chains in rolled metal sheets, covering the manufacturing process chain, microstructural features, crystallographic texture, and the anisotropy of functional properties. To ensure a high level of semantic interoperability, the models are aligned with Basic Formal Ontology (BFO) through the Platform MaterialDigital Core Ontology (PMDco 3.0)²⁰, a BFO-aligned domain-level ontology for MSE. The scope of the ontology is defined through competency questions (CQs) formulated in collaboration with domain experts and through a literature review. The coverage of the terminological box (TBox) is evaluated against the CQs using SPARQL Protocol and RDF Query Language (SPARQL)²¹ with a synthetic exemplary assertion box (ABox). The presented semantic models are implemented as NOES-Onto, an application-level ontology that focuses on the PSP dependencies of non-oriented electrical steels (NOES), which have been extensively investigated in the literature^{22,23}. While NOES-Onto is designed for the specific material class, the introduced design patterns and logical axioms are applicable more broadly to rolled metal sheets, establishing a reusable semantic foundation for PSP-oriented knowledge representation in the metal rolling domain. The presented semantic models enable systematic data integration, knowledge reuse, and inference

of implicit domain knowledge, and provide a foundation for the data-driven optimization of the performance of rolled metal sheets.

The remainder of the paper is structured as follows. Section [Related work](#) reviews advances in ontology development in the MSE domain. Section [Ontology development methodology](#) describes the selected methodology for the ontology development, defines the scope of the present semantic models through formulated competency questions, and briefly describes the imported ontologies. Section [Technical implementation](#) describes the technical implementation of NOES-Onto and reports ontology metrics. Section [Semantic models of the Process-Structure-Properties dependencies of rolled metal sheets](#) presents the semantic models in detail. Section [Usage scenarios](#) evaluates TBox coverage against the formulated CQs through usage scenarios, including an inference-based validation on a real EBSD dataset. Section [Discussion](#) discusses the capabilities and limitations of the present semantic models, and Section [Conclusions and outlook](#) concludes with an outlook on future work.

Related work

Ontologies in material science domain

The number of ontologies in the MSE domain has grown substantially in recent years, indicating the need for formal, machine-actionable, and interoperable knowledge representation in materials research. For example, MatPortal²⁴, an ontology repository for materials science, currently hosts 40

ontologies, many of which exhibit overlapping scope and vary in maintenance status. Within the German materials science community, the NFDI-MatWerk initiative²⁵ develops a materials science knowledge graph (MSE-KG)²⁶ as a shared semantic infrastructure for heterogeneous MSE datasets, including experimental results, simulation data, and scientific literature. While MSE-KG provides a general-purpose semantic layer for integrating structured and unstructured materials data, it does not address the formal axiomatization of PSP dependencies. De Baas et al.²⁷ assessed 43 MSE domain-level ontologies based on their alignment with top-level ontologies, such as BFO, Elementary Multiperspective Material Ontology (EMMO)²⁸, SemanticScience Integrated Ontology (SIO)²⁹, and Suggested Upper Merged Ontology (SUMO)³⁰. Only 10 of the reviewed ontologies were aligned with BFO, 21 adopted EMMO, and 4 had no top-level alignment²⁷, emphasizing the fragmented state of ontological alignment in MSE. Similarly, Norouzi et al.³¹ reviewed 60 ontologies from the MSE domain and evaluated them based on their alignment with top-level ontologies such as Provenance Ontology (PROV-O)³², BFO, SUMO, EMMO, and Descriptive Ontology for Linguistic and Cognitive Engineering (DOLCE)³³, as well as structural metrics and formulated quality requirements. In this study, only 10 ontologies were based on BFO. Nasrabadi et al.³⁴ argued that BFO-alignment is particularly advantageous for formal vocabularies in the MSE domain due to its well-structured taxonomy and querying performance. Beyond querying performance, BFO is standardized under ISO/IEC 21838-2:2021³⁵ and serves as the upper-level foundation of the Industrial Ontologies Foundry (IOF)³⁶, ensuring long-term stability, recognition in both academic and industrial contexts, and interoperability with the broader digital manufacturing domain. While EMMO²⁸ is a widely adopted alternative, its more complex axiomatization and the lack of ISO standardization pose practical challenges for industrial and cross-domain usage.

Several ontologies have been developed for the steel manufacturing process^{37,38}. Beden et al.³⁷ introduced a Steel Cold Rolling ontology (SCRO) to support the implementation of Industry 4.0³⁹ in steel plants. Cao et al.³⁸ presented the Common Reference Ontology for Steelmaking (SROS) and validated it through a cold rolling use case at Tata Steel with a focus on Industry 4.0 implementation. Although important for Industry 4.0 integration, both SCRO and SROS primarily focus on the semantic description of machinery control rather than the PSP dependencies of materials. Roters et al.⁴⁰ introduced StahlDigital-Ontology, which provides the foundation for the FAIR description of experimental and simulation data in steel production. Despite being more material-centric than SCRO and SROS, StahlDigital-Ontology still lacks the formal axiomatization required to support automated inference of PSP dependencies. Furthermore, none of SCRO, SROS, or StahlDigital-Ontology is aligned with BFO, limiting interoperability with the IOF³⁶ and the broader BFO-aligned ontology ecosystem. This highlights a gap in the formal, interoperable, and logically rigorous semantic description of rolling processes and the resulting PSP dependencies of metal sheets.

Despite the growing number of formal vocabularies in the MSE domain, no ontology addressed the PSP dependencies of rolled metal sheets in a formally rigorous, BFO-aligned semantic framework. Existing MSE ontologies either operate at a level of generality insufficient to capture manufacturing processes, microstructural features, crystallographic texture, and resulting material properties or focus on process control rather than material performance. The present work bridges this gap by providing a formal, BFO-aligned framework that encodes the PSP dependencies of rolled metal sheets and supports FAIR data management, semantic reasoning, and data-driven methods for material optimization.

Ontology development

Ontology engineering is a knowledge-intensive process that requires input from domain and ontology experts⁴¹. The development of the present semantic models follows the ontology development scenarios from the NeOn methodology⁴². While Scenario 1: From specification to implementation is necessary for every ontology development, the remaining 8 scenarios can be leveraged depending on the reuse of ontological and non-ontological resources as well as ontology design patterns (ODPs) and requirements on ontology structure and localization⁴². The detailed use of the NeOn scenarios is described in Section [Ontology development methodology](#).

The requirements for a new ontology can be specified through various approaches, including identifying a motivating scenario or purpose, conducting a feasibility study, and formally specifying requirements via CQs⁴³. CQs represent questions in natural language that the ontology must address, thereby guiding the formalization of classes, object properties, and logical axioms. The formulated CQs can subsequently be transformed into SPARQL queries to formally evaluate the coverage of the developed TBox against the defined scope^{44,45}. In the present work, CQs are adopted as the primary methodology for defining the modeling scope, as detailed in Section [Modeling scope](#).

As ontology development goes beyond formalization of domain-relevant terms, the design decisions developed within the new ontology are formalized in the form of ODPs, i.e., reusable modeling solutions for solving recurring modeling challenges in knowledge graph design⁴⁶. ODPs that are widely accepted by the Semantic Web community can be found on ODP portal⁴⁷. Presutti et al.⁴⁸ suggested an eXtreme Design methodology for ontology development that selects and reuses existing ODPs based on the formulated CQs, corresponding to Scenario 7 of the NeOn methodology⁴². The evaluation of the eXtreme Design methodology showed that reusing ODPs improves ontology quality and usability and mitigates modeling mistakes⁴⁹.

Ontology quality can be assessed at multiple levels, including alignment to the formulated requirements, sufficient annotation of introduced resources, logical soundness of axioms, and alignment with FAIR principles. While the first can be evaluated through SPARQL queries based on the CQs and the feedback from ontology users, the latter three can be assessed through common tooling. For example, the Ontology Pitfall Scanner (OOPS!) analyses ontologies for 41 pitfalls across 3 severity levels⁵⁰. Alternatively, the `report` command from the ROBOT ontology management

tool performs similarly to OOPS! quality control on annotation and logical soundness, returning violations at 3 severity levels⁵¹. The Ontology Pitfall Scanner for FAIR Principles (FOOPS!) assesses alignment with FAIR principles based on 24 checks⁵².

Ontology development methodology

The present semantic models are developed utilizing selected scenarios from NeOn methodology⁴². First, the modeling scope is defined via CQs formulated from interviews with domain experts, corresponding to Scenario 1: From specification to implementation. Subsequently, Scenario 4: Reusing and re-engineering ontological resources is utilized to import resources from selected ontologies. Scenario 7: Reusing ontology design patterns is adopted to follow modeling design decisions developed within PMDco 3.0²⁰ and Crystallography Ontology (Cryo)⁵³. Finally, the semantic models are developed in a modular manner inspired by ODP approach⁴⁶ to address individual aspects of the PSP dependencies of rolled metal sheets and support reusability. However, neither imported nor introduced design patterns are officially published on the ODP portal⁴⁷.

Modeling scope

In the present work, CQs are adopted as the primary methodology for defining the modeling scope. As the semantic models are validated for the NOES use case, requirements were elicited through semi-structured interviews with 14 industry-affiliated researchers and engineers specializing in NOES. Subsequently, recurring topics across respondents were consolidated into a preliminary list of CQs. Duplicate and overlapping questions were merged, and the resulting set was organized into three categories corresponding to the PSP paradigm. The interview questions and a summary of the coding procedure are provided as supplementary material.

The initial CQ set was subsequently extended through a literature review guided by the domain expertise of the authors. Publications on NOES were grouped thematically, covering the influence of chemical composition and manufacturing parameters on microstructure, crystallographic texture, and the anisotropy of functional properties. Topics that were underrepresented in the interview responses were formalized into additional CQs. This supports broad coverage of the scope, reflecting both established industrial practices and current research challenges.

The complete list of the formulated CQs is given in Table 1, where the source (industry or literature) is specified. The questions are divided into three categories: manufacturing, assessment of microstructure and crystallographic texture, and assessment of functional properties. These categories directly correspond to the Process, Structure, Property features of the PSP paradigm.

In the manufacturing category, the processes relevant to the production of NOES are considered. The chemical composition is evaluated as an input characteristic for a casting process (CQ1). Manufacturing history and process parameters of individual manufacturing steps, such as temperature, duration, number of rolling passes, and thickness reduction, are assessed in CQ2 and CQ3,

respectively. The processing of semi-finished products, i.e., coated and cut NOES sheets, is addressed in CQ4 and CQ5.

The second category focuses on the microstructure and crystallographic texture of NOES sheets at different manufacturing stages. CQ6 to CQ8 address the grain size, presence of metallic and non-metallic inclusions, and volume fractions of characteristic crystallographic texture components. Additionally, the presence and location of deformed structures, e.g., shear and dislocation bands, after heat treatment or rolling, is assessed in CQ9, which falls outside the scope of the current version.

The third category highlights magnetic and mechanical properties, as these are of particular interest for the NOES use case. CQ10 addresses the effect of chemical composition on material properties. The dependence of the magnetic and mechanical properties of NOES sheets on external conditions, such as temperature, frequency, strength of the applied magnetic field, and mechanical load, is considered in CQ11. CQ12 addresses material selection based on functional performance under given operation conditions. Furthermore, CQ13 addresses the trade-off between magnetic and mechanical properties in NOES. Lastly, CQ14 evaluates the discrepancy between simulated and measured values of a given NOES property, though it falls outside the scope of the current version.

CQs marked as out of scope (CQ4, CQ5, CQ9, CQ14) address aspects whose formal description requires ontological infrastructure beyond the current implementation. Their integration is planned for future versions of the semantic models, as discussed in Section [Out-of-scope competency questions](#).

Overall, the individual CQs listed in Table 1 can be combined to elucidate the influence of manufacturing steps on the resulting microstructure of NOES and, subsequently, the performance of the material under given conditions. For example, a SPARQL query featuring CQ1 and CQ7 reveals the influence of chemical composition on the formation of inclusions, while a combination of CQ7 and CQ10 highlights the effect of inclusions on the mechanical and magnetic performance of NOES. Alternatively, a query with CQ3 and CQ8 emphasizes the influence of manufacturing process parameters on the resulting crystallographic texture, while CQ8 combined with CQ11 aims to identify the optimal texture under given operating conditions.

While the resulting CQs are formulated in the context of NOES, the topics they cover, i.e., manufacturing process chains, microstructural characterization, crystallographic texture, and the anisotropy of functional properties, are representative of the broader PSP space of rolled metal sheets.

Imported ontologies

Reusing existing ontologies is a common practice in ontology engineering⁵⁹. It promotes semantic interoperability across domains, enables the inheritance of logical rigor from mature top-level ontologies, supports modular ontology development, and avoids redundant formalization of terms. The present semantic models are aligned with BFO through the principal imported ontologies PMDco 3.0²⁰, CryO⁵³, and Tensile Testing Ontology (TTO)⁶⁰, enabling direct reuse

Table 1. Competency questions categorized by three topics: manufacturing, assessment of microstructure and crystallographic texture, and assessment of functional properties.

ID	Question	Source	In scope (v1)
Manufacturing			
CQ1	What is the chemical composition of material X?	Industry, Literature ^{7,54}	Yes
CQ2	What is the manufacturing history of the NOES sheet X?	Literature ^{55,56}	Yes
CQ3	What are attributes of a processing step X of a material Y?	Literature ^{57,58}	Yes
CQ4	Which stamping parameters must be used for cutting of NOES sheets, if it has a coating X?	Industry	No
CQ5	What is the number of sheets in a stack with the height X, if the thickness of a single sheet is Y and its flatness deviation is Z?	Industry	No
Assessment of microstructure and crystallographic texture			
CQ6	What is the average grain size of a material X after all manufacturing steps?	Literature ^{7,54}	Yes
CQ7	Are any metallic / non-metallic inclusions present in the microstructure of material X?	Literature ^{7,54}	Yes
CQ8	What are the volume fractions of characteristic texture components in a fully processed sheet?	Literature ^{56,58}	Yes
CQ9	Are any deformed regions present in the microstructure after the manufacturing step X?	Literature ^{7,56}	No
Assessment of microstructure and crystallographic texture			
CQ10	What is the value of material property X based on the provided chemical composition?	Industry	Yes
CQ11	Which value of a property X does the material Y have under given temperature, frequency, mechanical load, etc.?	Industry	Yes
CQ12	Which material is used in an application with a set of environment parameters X, e.g., temperature, frequency, mechanical load, etc., which material has the best magnetic performance?	Industry	Yes
CQ13	If a given material has a set of mechanical properties X (for high-loading application, e.g., rotor), what total magnetic losses does it have?	Industry	Yes
CQ14	What is the difference between the simulation-derived value of a property X for a material Y, compared to the measured value?	Industry	No

of resources without additional alignment layers. To incorporate essential concepts from the MSE domain, e.g., a taxonomy of materials, manufacturing processes, and material properties, PMDco 3.0²⁰, an MSE-specific mid-level semantic framework developed within the MaterialDigital initiative⁶¹, is imported. While BFO is originally formalized in first-order logic (FOL), PMDco 3.0 is built on its description logic (DL) formalization, enabling automated reasoning at the cost of reduced expressivity compared to the full FOL specification. TTO and CryO, both built on PMDco 3.0, are further imported, providing formalizations of the tensile testing process and crystallographic concepts, respectively. Lastly, selected terms from Units Ontology (UO)⁶² and Quantities, Units, Dimensions and Types (QUDT)⁶³ are imported to ensure an interoperable representation of units of physical quantities.

As ontologies on which the present semantic models are built use opaque numeric URIs following the OBO identifier pattern, resources are denoted by combining the abbreviation of a source ontology as a prefix (e.g., `noes:`, `pmd:`, `bfo:`) with their human-readable *rdfs:label* rather than their underlying numerical URIs. Note that while this notation

intentionally includes whitespace for reading fluidity, it serves strictly as a typographic presentation in this text and does not constitute syntactically valid URI or CURIE notation. The following notations are used for addressing ontology resources:

- Resources of type `OWL:CLASS` are given in **bold**
- Resources of type `OWL:OBJECTPROPERTY` are given in *italic*
- Resources of type `OWL:NAMEDINDIVIDUAL` are given in monospace and use `ex:` (`http://example.org/`) prefix

In the logical axioms presented in the following sections, namespace prefixes are omitted for clarity.

Platform Material Digital Core Ontology (PMDco 3.0)

PMDco 3.0 is a mid-level ontology for the MSE domain, which is built on BFO and reuses resources from other supporting ontologies, such as the Relation Ontology (RO)⁶⁴, Information Artifact Ontology (IAO)⁶⁵, Ontology for Biomedical Investigations (OBI)⁶⁶, and the Chemical Entities of Biological Interest (ChEBI)⁶⁷ ontology. PMDco

3.0 provides classes, object properties, and design patterns for the semantic description of chemical composition, material properties, measurement assays, and manufacturing processes. This section describes ODPs from PMDco 3.0 that are adopted and, where necessary, extended for the semantic modeling of rolled metal sheets.

Manufacturing process and temporally qualified continuants A manufacturing process in PMDco 3.0 is characterized by specified inputs and outputs, represented by physical objects, and corresponding process attributes that define the conditions under which the process takes place. An exemplary KG describing a manufacturing process is shown in Figure 2, and its modeling is based on the axioms and design patterns provided by PMDco 3.0. The inputs and outputs are simultaneously instances of **bfo:object** and **pmd:material**, the former emphasizes physical boundedness, whereas the latter is demarcated by any physical discontinuities²⁰. Process attributes describe the conditions under which a process takes place and may refer to a quality of a process participant via *pmd:refers to*, e.g., the temperature attribute of a rolling process, which refers to the temperature of the rolled material during the process. The process attribute or the corresponding quality is specified by a scalar value specification.

Within a manufacturing process chain, individual processes are temporally ordered via *bfo:precedes* relation, enabling sequential querying of the full process history. However, the temporal ordering of processes alone does not capture the evolution of material between stages. To reflect this evolution throughout the process chain, PMDco 3.0 adopts a concept of Temporally Qualified Continuants (TQCs) introduced in⁶⁸. Time-invariant qualities are assigned to the base individual, while qualities that evolve across the process chain are attributed to temporal individuals of a TQC class. Each TQC individual exists only during a specified temporal region and represents the state of a material or object at a given stage of the process chain. Leveraging TQCs addresses a fundamental limitation of OWL 2 DL, which does not support time-dependent class membership, i.e., the *rdf:type* of an individual is persistent throughout its existence. Each TQC individual has its own type assertion, allowing the same base material to be associated with different states and, therefore, different ontological classes, without violating OWL 2 DL type persistence.

Material properties and their measurements BFO distinguishes between specifically dependent continuants (SDCs) that require a process for their realization and those that characterize independent continuants without any realization in a process. PMDco 3.0 follows this distinction by classifying material qualities, which are intrinsic to the existence of the material, under **bfo:quality**, and the material properties, which require a process for realization, under **bfo:realizable entity**. For instance, soft magnetic properties require the application of a magnetic field, whereas material qualities such as chemical composition, average grain size, and crystallographic texture describe the current state of the material. This distinction supports the formal resolution of structure-property dependencies of materials. Regardless of the type of SDC of a material, its value can be determined in an assay, as shown in Figure 3, where an assay measures

some characteristic of the material and outputs the value of the property.

Crystallography Ontology (CryO) CryO is an application-level ontology that extends PMDco 3.0 with classes, object properties, and logical axioms tailored for the semantic description of crystallographic entities, such as directions, planes, and families of symmetry-equivalent directions and planes⁵³. The adoption of CryO in the present semantic models is motivated by the influence of crystallographic texture on the anisotropy of the functional properties of rolled metal sheets. As illustrated in Figure 4, CryO enables automatic inference of the symmetry-equivalent family of Miller indices for a crystallographic plane or direction, given an assertion of a lattice system. For example, it is inferred that a (0 1 1) plane in a cubic system belongs to the {1 1 0} family. This inferential capability is leveraged in the present semantic models, as detailed in Section [Formal description of crystallographic texture and its quantitative characteristics](#).

Tensile Testing Ontology (TTO) TTO is an application-level ontology that extends PMDco 3.0 with classes for the semantic description of the tensile testing process and associated material properties⁶⁰. Given the limited overlap between tensile testing and the scope of the present semantic models, only a subset of classes for mechanical properties and geometric features of tensile specimens is imported from TTO, ensuring consistency with the broader ontology stack while avoiding redundant formalization. These classes directly support the representation of mechanical properties addressed in CQ11, CQ12, and CQ13.

Unit ontologies To formally express units of material properties and process parameters, NOES-Onto imports selected individuals from UO⁶², and QUDT⁶³. The primary advantage of UO is its alignment with BFO, ensuring semantic interoperability with other BFO-aligned ontologies. However, not all units relevant to the NOES domain are present in UO. Therefore, the missing units are imported from QUDT and manually aligned with the UO-based taxonomy to ensure consistent unit representation across the present semantic models.

Technical implementation

The present semantic models are implemented in NOES-Onto, which is built and curated using the Ontology Development Kit (ODK), a containerized toolkit for managing core tasks in ontology development, including dependency resolution, quality control, and release preparation⁶⁹. To facilitate independent development and maintenance, NOES-Onto is structured into modular components: external imports alongside thematic modules covering manufacturing processes, materials, characterization, and crystallographic texture. Through the ODK pipeline, NOES-Onto is provided in three distinct release artifacts: full (fully merged with all external dependencies), base (local axioms only), and basic (a filtered version optimized for standard applications). This ensures compatibility across diverse deployment contexts and reasoning tasks.

Ontology metrics NOES-Onto introduces 159 new classes and 4 new object properties for the BFO-aligned semantic description of PSP dependencies of rolled metal sheets,

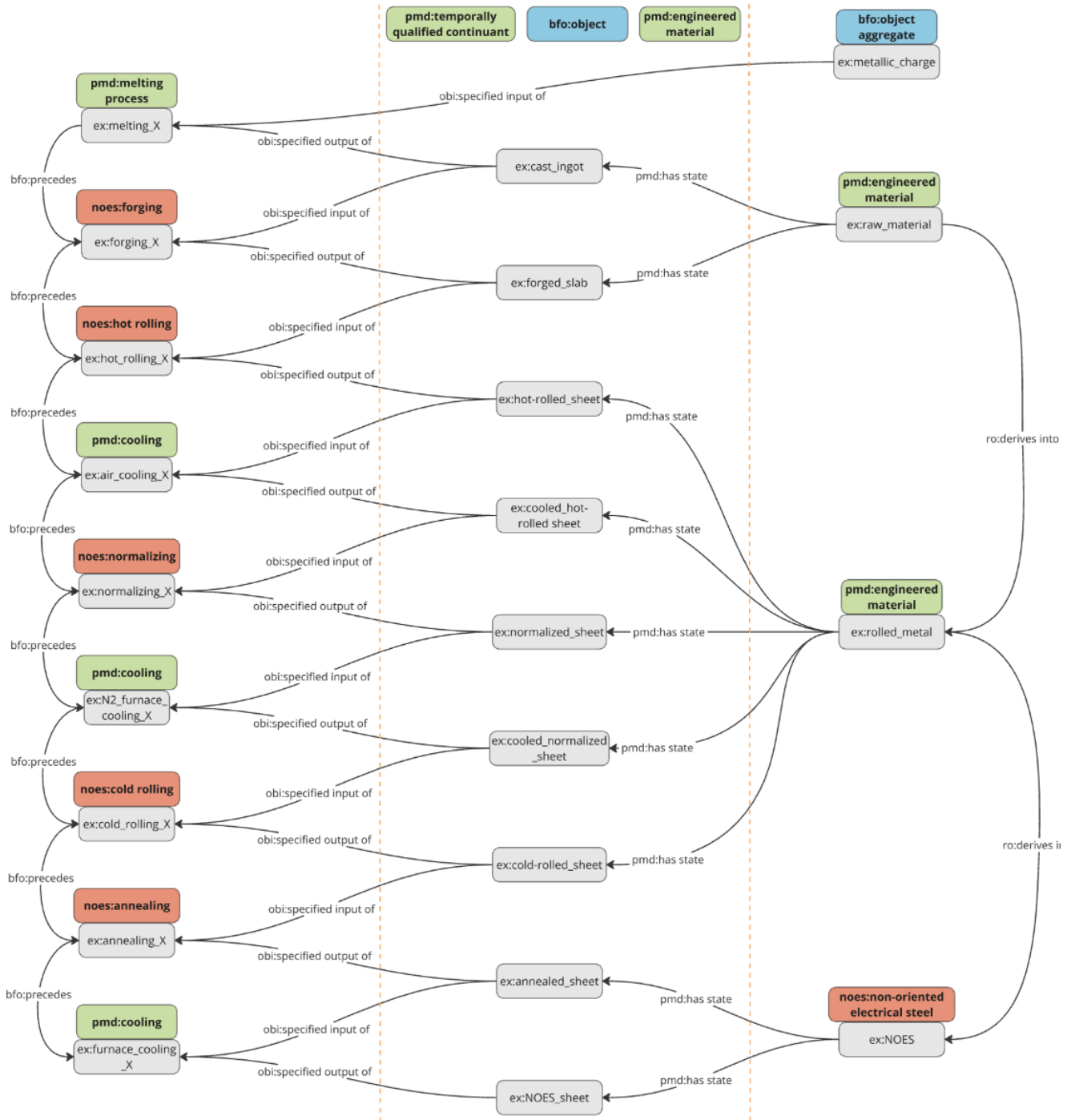


Figure 5. Semantic modeling of a conventional manufacturing process chain of rolled metal sheets. The orange dashed lines indicate TQC individuals, each of which is simultaneously an instance of **pmd:temporally qualified continuant**, **bfo:object**, and **pmd:engineered material**; the corresponding *rdf:type* relations are omitted for clarity. Temporal ordering between processes is expressed via **bfo:precedes**. The analogous temporal sequencing between TQC individuals can be expressed using the corresponding design pattern from PMDco 3.0, but is omitted here for clarity. Every TQC individual is related to its base individual via **pmd:has state** and serves as a specified input or output to a manufacturing process. The emergence of a new base individual after hot rolling reflects the qualitative change in the material introduced by the rolling reference frame, while a third base individual represents the fully-processed material, e.g., **noes:non-oriented electrical steel**. The relation between base individuals is formalized via **ro:derives into**.

plastic deformation causes randomly oriented grains to rotate, resulting in a preferred grain orientation relative to the reference frame of the rolled sheet. This reference frame is defined by rolling and transverse directions (RD and TD, respectively), which together with the RD define a rolling plane (RP), and a normal direction (ND) (Figure 7a). A formal description of this reference frame is essential for

the semantic modeling of crystallographic texture and the resulting anisotropy of functional properties.

The formalization of these characteristic directions starts with the introduction of necessary classes: **noes:rolled sheet direction** and its subclasses **noes:rolling direction**, **noes:transverse direction**, and **noes:normal direction**. These are modeled as subclasses of **bfo:flat line**, i.e.,

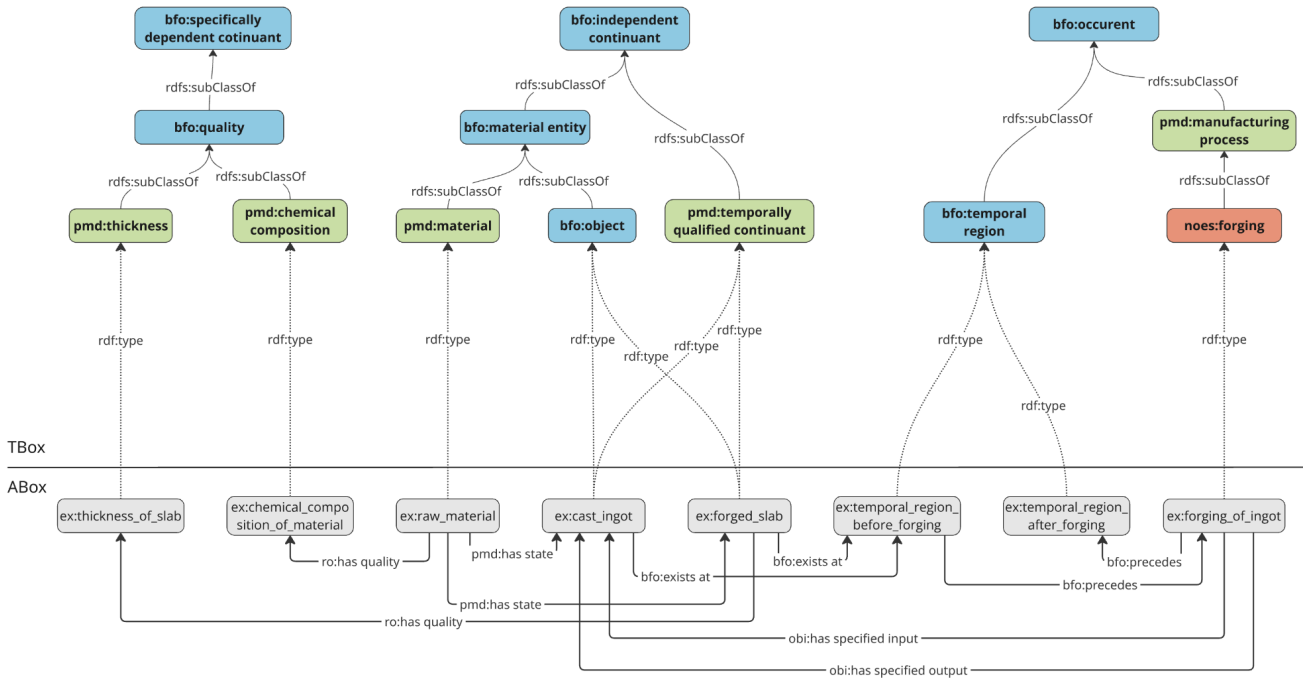


Figure 6. Semantic modeling of qualities of materials featuring TQCs, using a forging process as an example (TBox/ABox view): chemical composition is a time-invariant quality and, therefore, is assigned to the base individual `ex:raw_material`, while thickness of a cast ingot is reduced during a forging process and is assigned to the output TQC individual `ex:forged_ingot`. Each TQC individual is anchored to a temporal region via `bfo:exists at`; the temporal ordering of states is then expressed via `bfo:precedes` between the temporal regions and the forging process.

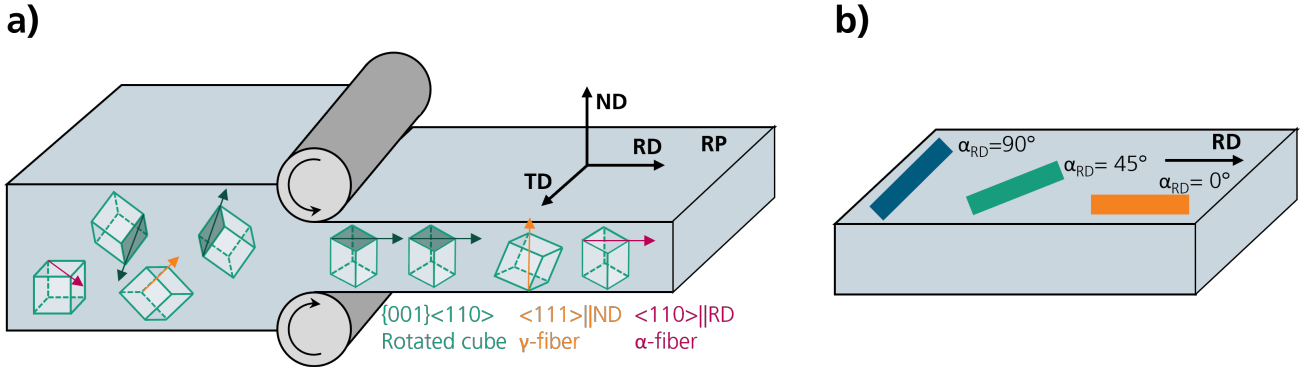


Figure 7. a) Schematic of a rolling process, where randomly oriented grains exhibit a preferred orientation with respect to the rolling reference frame, defined by rolling, transverse, and normal directions (RD, TD, and ND, respectively), as well as the rolling plane (RP). The preferred grain orientations are represented by rotated cube texture component $\{001\}\langle 110 \rangle$ (green), γ -fiber $\langle 111 \rangle \parallel \text{ND}$ (orange), and α -fiber $\langle 110 \rangle \parallel \text{RD}$ (pink). b) Specimens cut at 0° , 45° , and 90° to RD in RP, used to investigate the anisotropy of functional properties.

one-dimensional immaterial entities whose location is determined in relation to a material entity, i.e., a rolled sheet. Additionally, **noes:longitudinal direction** (LD) is introduced as a superclass of **noes:rolling direction** and **noes:transverse direction**, representing any direction contained within RP. These entities are related by the following geometric constraints: RD and TD are parts of the RP; RP, and consequently, both RD and TD, are normal to ND. Thus, three new object properties are introduced to express these geometric relations: **noes:geometrically related** along with its subproperties **noes:parallel to** and **noes:normal to**. To support logical reasoning, Axioms 1 are defined. First, Axioms 1a and 1b constrain the domain and range of introduced object properties to **bfo:independent**

continuant as only these types of BFO entities can exhibit geometric relations with respect to each other. Second, **noes:parallel to** is symmetric and transitive (Axioms 1c and 1d), while **noes:normal to** is symmetric (Axiom 1e). Lastly, a property chain Axiom 1f encodes the geometric rule that if entity X is normal to Y, and Y is parallel to Z, then X is normal to Z.

$$\exists \text{geometrically related.} \top \sqsubseteq \text{independent continuant} \quad (1a)$$

$$\top \sqsubseteq \forall \text{geometrically related.independent continuant} \quad (1b)$$

$$\text{parallel to} \sqsubseteq \text{parallel to}^- \quad (1c)$$

$$\text{parallel to} \circ \text{parallel to} \sqsubseteq \text{parallel to} \quad (1d)$$

$$\text{normal to} \sqsubseteq \text{normal to}^- \quad (1e)$$

$$\text{normal to} \circ \text{parallel to} \sqsubseteq \text{normal to} \quad (1f)$$

The geometric relations between characteristic directions and RP are expressed as necessary conditions given in Axioms 2. The RP is normal to the ND (Axiom 2a). The LD (and therefore, RD and TD) is part of the RP and parallel to it, as given in Axioms 2b and 2c, respectively. Finally, Axiom 2d states that the RD is normal to the TD. As the RD, TD, ND, and RP define the reference frame of the rolled sheet, a formal relation between these immaterial entities and the sheet is defined via *ro:located in*. The introduced axioms enable inference of implicit geometric relations within the rolling reference frame, e.g., orthogonality between RD and ND and between TD and ND, and provide the formal basis for the semantic description of crystallographic texture and property anisotropy.

$$\text{rolling plane} \sqsubseteq \exists \text{normal to. normal direction} \quad (2a)$$

$$\text{longitudinal direction} \sqsubseteq \exists \text{part of. rolling plane} \quad (2b)$$

$$\text{longitudinal direction} \sqsubseteq \exists \text{parallel to. rolling plane} \quad (2c)$$

$$\text{rolling direction} \sqsubseteq \exists \text{normal to. transverse direction} \quad (2d)$$

In the current version of developed semantic models, it is assumed that RD remains constant throughout subsequent manufacturing steps, particularly during cold rolling. This is a modeling simplification, as ongoing research investigates the influence of changes of RD during the cold-rolling process on the crystallographic texture and magnetic properties of NOES⁷¹. Nevertheless, the TQC-based modeling approach provides the necessary logical rigor to formally represent the change in RD across manufacturing states, but its formal representation is deferred to future versions.

Semantic description of specimen cutting at an angle to the RD Specimens of rolled metal sheets are often cut at an angle to the RD in the RP to investigate the anisotropy of their functional properties, as shown in Figure 7b. To express the angle between an arbitrary direction in RP and RD, we introduce a class **noes:angle to rolling direction** as a subclass of **bfo:relational quality**. The choice of the parent class is motivated by its semantics, as relational qualities in BFO simultaneously depend on two bearers. The new class has a necessary condition expressed in Axiom 3. Here, the angle to the RD is a relational quality between two fiat lines: the RD is located in the material, and the LD is located in the cut specimen. This distinction leverages the PMDco material/object duality to formally separate the reference direction of the material from the cutting direction of the specimen. As both LD and RD are defined as parts of RP (Axiom 2b), the angle is necessarily defined between two directions within the RP. An exemplary KG illustrating the design pattern for a cutting process at 45° to RD is given in Figure 8.

$$\begin{aligned} \text{angle to rolling direction} &\sqsubseteq \\ &(\exists \text{relational quality of.} (\\ &\text{longitudinal direction} \sqcap \exists \text{located in. object})) \\ &\sqcap (\exists \text{relational quality of.} (\\ &\text{rolling direction} \sqcap \exists \text{located in. material})) \end{aligned} \quad (3)$$

Assessment of anisotropy of functional properties

Functional properties of rolled metal sheets exhibit anisotropy within the RP, arising from the preferred grain orientation developed during hot and cold rolling processes. The assessment of the anisotropy of properties is carried out by using specimens cut from the whole sheet (as shown in Figure 8) as input to the corresponding measurement processes. The type of a measured property does not change with the orientation of the specimen relative to RD, e.g., total magnetic power loss remains semantically the same, but its magnitude varies, necessitating a

formal framework to distinguish such values obtained at different orientations. A necessary and sufficient condition expressed in Axiom 4 enables inference of any property measured at a given direction to RD, if a specimen, serving as a specified input to the assay, has a relational quality **noes:angle to rolling direction** defined by numerical value X . For instance, as illustrated in Figure 9, a class **noes:total magnetic power loss in the rolling direction** is inferred for an instance of **noes:total magnetic power loss**, if the property is measured on a specimen cut at 0° to RD in RP.

property at angle X to RD $\equiv$

$$\begin{aligned} \text{property} &\sqcap \exists \text{characteristic measured by assay.} (\\ &\text{assay} \sqcap \exists \text{has specified input.} (\text{object} \sqcap \exists \text{location of.} (\\ &\text{longitudinal direction} \sqcap \exists \text{has relational quality.} (\\ &\text{angle to rolling direction} \sqcap \exists \text{specified by value.} (\\ &\text{scalar value specification} \\ &\sqcap \exists \text{has specified numeric value.} \{X\} \} \} \} \} \} \} \end{aligned} \quad (4)$$

Formal description of crystallographic texture and its quantitative characteristics

A formal description of crystallographic texture is essential to address CQ8 and establish the causal link between texture and anisotropy of functional properties. To achieve this, logical axioms are introduced that enable the automatic inference of crystallites contributing to texture components and fibers. Subsequently, a design pattern is proposed for the semantic modeling of the volume or area fractions of these texture features, as quantified by post-processing of X-ray diffraction (XRD) or electron backscatter diffraction (EBSD).

Axiomatisation of crystallographic texture Crystallographic texture is characterized by a family of equivalent crystallographic directions $\langle uvw \rangle$ of crystallites being parallel to either RD or ND of a rolled sheet, thereby defining texture fibers⁷². The exemplary texture fibers are shown in Figure 7a, including the γ -fiber, characterized by $\langle 111 \rangle$ crystallographic directions oriented parallel to ND, and the α -fiber, defined by $\langle 110 \rangle$ directions oriented parallel to RD. When a family of equivalent crystallographic planes $\{hkl\}$ additionally aligns with the RP, a discrete texture component is defined. For example, the rotated cube texture component (Figure 7a) is characterized by $\langle 110 \rangle$ directions oriented parallel to the RD and $\{001\}$ planes oriented parallel to the RP. However, the orientation space of the actual microstructure is continuous, i.e., there are infinitely many possible orientations, which are rarely oriented perfectly to fulfill the requirements of $\langle uvw \rangle$ oriented parallel to the RD (or ND) and $\{hkl\}$ oriented parallel to the RP. A misorientation angle between the orientation of an actual crystallite and the ideal $\langle uvw \rangle \{hkl\}$ orientation is defined as the minimum rotation angle required to align the two orientations⁷². If the magnitude of the misorientation angle falls below the threshold (conventionally 15°), the crystallite is considered to contribute to the specified texture component or fiber.

To collectively describe the crystallites that contribute to a given texture, a class **noes:grain population** is introduced as a subclass of **bfo:object aggregate**. These crystallites are spatially distributed throughout the material, and their membership in the grain population is determined by grain orientation criteria rather than physical adjacency. Therefore, **noes:grain population** cannot be classified as either a connected or a disconnected object aggregate in the PMDco 3.0 taxonomy. Consequently, crystallographic texture is modeled as a quality of a grain population. Axiom 5 formalizes this relation using both existential and universal restrictions, ensuring that the bearer of a crystallographic texture is a collection of

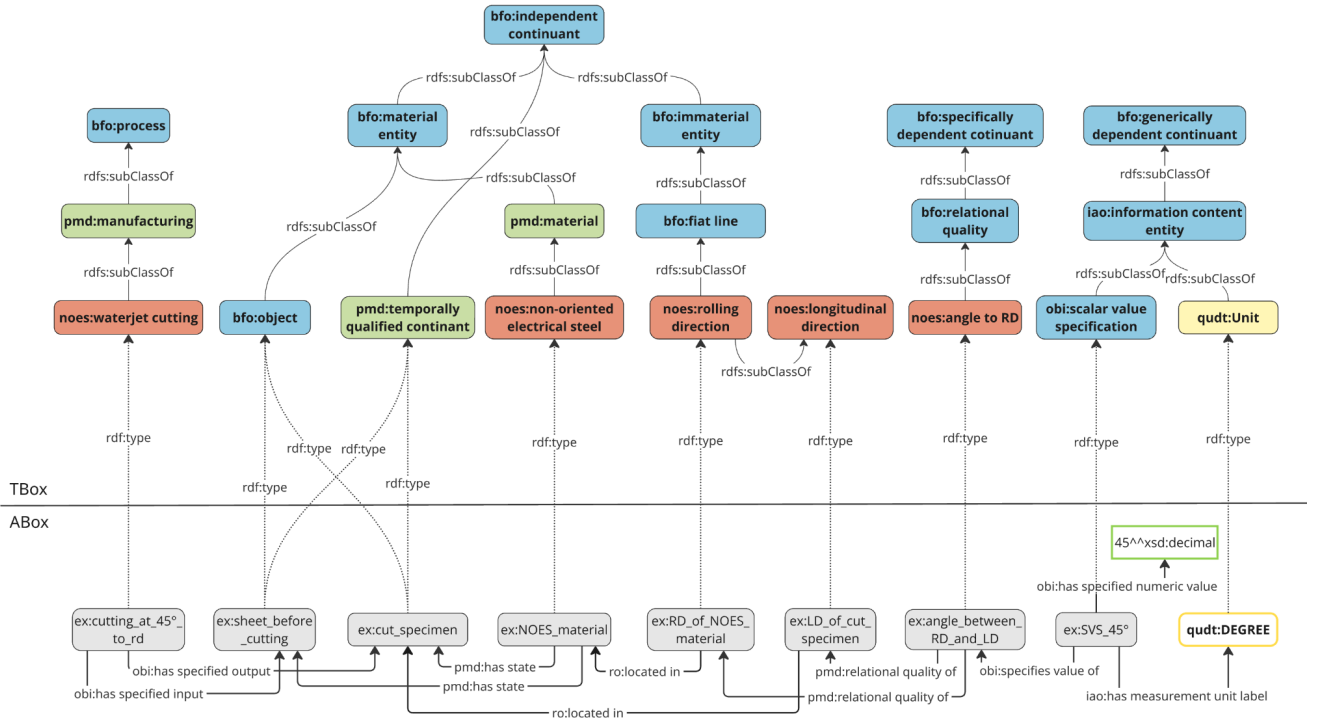


Figure 8. Design pattern for the semantic description of cutting rolled metal sheets at an angle to RD (TBox/ABox view). The cutting process has TQC individuals as input and output. The LD, i.e., an arbitrary direction within the RP, is located in the cut specimen. The RD is located in the base individual of an NOES material. The angle between LD and RD is defined as 45°.

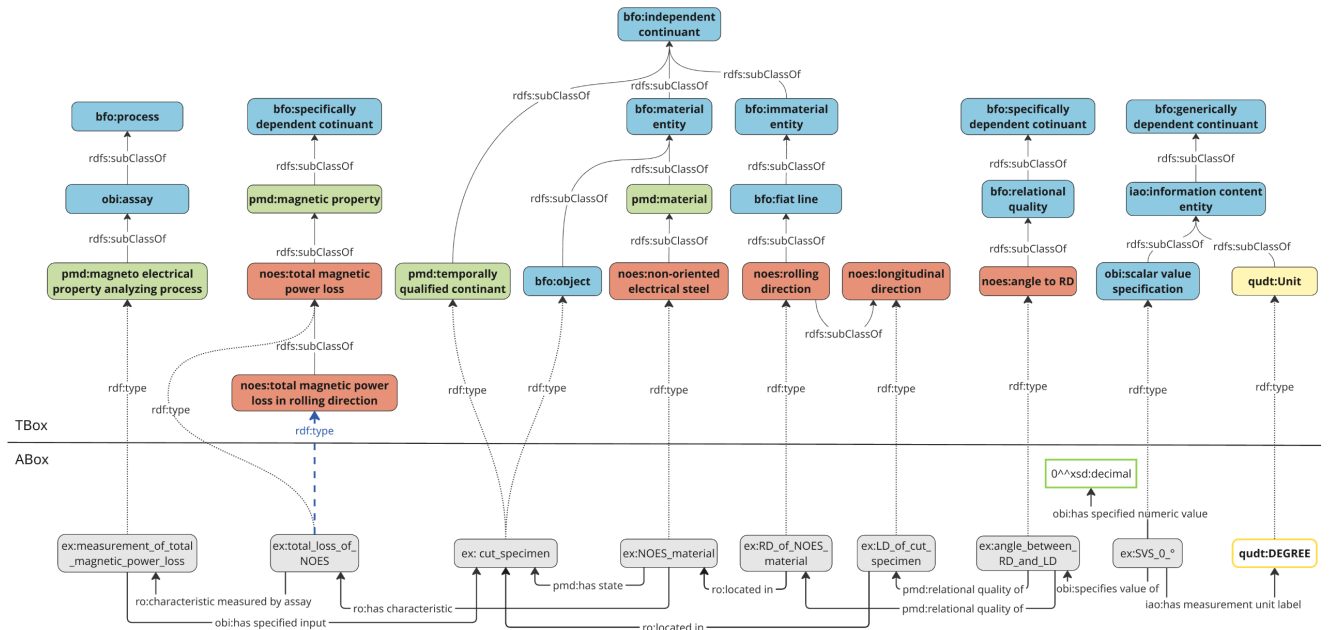


Figure 9. Design pattern for the inference of a direction-specific property class based on the anisotropy axiom (TBox/ABox view). The blue dashed line indicates an inferred triple. The assay measures the total magnetic loss in a specimen cut parallel to the RD of the sheet, i.e., the angle between the LD of the specimen and the RD of the material is 0°. Based on the necessary and sufficient condition expressed in Axiom 4, the individual of the measured property is inferred to be of type **noes:total magnetic power loss in the rolling direction**.

similarly oriented crystallites.

crystallographic texture $\sqsubseteq$

$$\exists \text{quality of.grain population} \forall \text{quality of.grain population} \quad (5)$$

To infer that a grain contributes to the characteristic texture component or fiber, logical axioms combined with the Miller indices family inference provided by CryO via its property chain

axiom (Figure 4) are leveraged. First, an ideal grain orientation for a given texture component is formally defined through a necessary and sufficient condition, as given in Axiom 6. The axiom is decomposed into three parts: the first two focus on constraining the orientations of $\langle uvw \rangle$ directions and $\{hkl\}$ planes in the crystallite relative to the reference frame of the rolled sheet, and the third combines these constraints into an axiom defining a

crystallite whose orientation satisfies a specific texture component or fiber. In particular, Axiom 6a constrains the crystallographic direction denoted by $\langle uvw \rangle$ in the cubic system to be parallel to the RD. Similarly, Axiom 6b defines a constraint on the crystallographic plane $\{hkl\}$ being parallel to the RP. Finally, Axiom 6c defines a specific crystallite with ideal orientation as a location of these crystallographic directions and planes, i.e., whose orientation satisfies the definition of a specific texture component. For texture fibers where $\langle uvw \rangle$ is parallel to ND, the axioms are defined by replacing RD with ND in Axiom 6a. The axioms for crystallites that contribute to texture fibers are obtained by omitting the constraint on the RP in Axiom 6c.

$$\begin{aligned} \Phi_{RD} &\equiv \text{crystallographic direction} \\ &\sqcap \exists \text{denoted by family under cubic symmetry.} \\ &\quad (\text{Miller indices } \sqcap \exists \text{has Miller indices.}\{\langle uvw \rangle\}) \quad (6a) \\ &\sqcap \exists \text{parallel to.} \\ &\quad (\text{rolling direction } \sqcap \exists \text{located in. material}) \end{aligned}$$

$$\begin{aligned} \Phi_{RP} &\equiv \text{crystallographic plane} \\ &\sqcap \exists \text{denoted by family under cubic symmetry.} \\ &\quad (\text{Miller indices } \sqcap \exists \text{has Miller indices.}\{\{hkl\}\}) \quad (6b) \\ &\sqcap \exists \text{parallel to.} \\ &\quad (\text{rolling plane } \sqcap \exists \text{located in. material}) \end{aligned}$$

$$\begin{aligned} \text{ideal crystallite with X orientation} &\equiv \text{crystallite} \\ &\sqcap \exists \text{location of. } \Phi_{RP} \quad (6c) \\ &\sqcap \exists \text{location of. } \Phi_{RD} \end{aligned}$$

To formally define the requirement for a crystallite to contribute to a given texture component, a class **noes:misorientation angle** as a subclass of **bfo:relational quality** is introduced. A crystallite contributing to the texture component or fiber is defined via a necessary and sufficient condition given in Axiom 7. The misorientation angle is defined between the actual crystallite and the reference crystallite with ideal orientation. An object property *ro:towards* is used between the misorientation angle and the crystallite with ideal orientation, as it relates a relational quality to an independent continuant other than its (primary) bearer. Additionally, it avoids cyclic reasoning that could arise if *pmd:relational quality of* were used bidirectionally with its inverse *pmd:has relational quality*. Following the conventional threshold of 15° ⁷², a crystallite is considered to contribute to the texture if the misorientation angle falls below this value.

$$\begin{aligned} \text{crystallite with X orientation} &\equiv \text{crystallite} \\ &\sqcap \exists \text{has relational quality. (misorientation angle} \\ &\quad \sqcap \exists \text{specified by value. (} \\ &\quad \exists \text{has measurement unit label. \{degree\}} \\ &\quad \sqcap \exists \text{has specified numeric value. (xsd:float} [\leq 15.0]) \text{))} \\ &\quad \sqcap \exists \text{towards. ideal crystallite with X orientation}) \quad (7) \end{aligned}$$

In practice, a crystallite with exactly the ideal orientation of a given texture component is unlikely to exist in the microstructure. Formally asserting an individual of a class of a crystallite with ideal orientation, i.e., the defined class from Axiom 6c, without a corresponding physical instance conflicts with the requirement of BFO that all instances of **bfo:continuant** persist in reality. However, under the Open World Assumption (OWA) of OWL 2 DL, it can be assumed that such a crystallite physically persists without specifying its microstructure or material.

Figure 10 presents an example of such inference using Axiom 7 for the cube $\{001\}\langle 100 \rangle$ texture component. The crystallite is inferred to be of type **noes:crystallite with cube texture orientation** as the misorientation angle of 9° falls below the 15° threshold.

Classes of specific crystallographic textures are introduced as subclasses of **pmd:crystallographic texture**, defined by existential and universal restrictions on the membership of the grain population, as given in Axiom 8, ensuring that all members of the grain population have the required orientation. NOES-Onto covers the characteristic textures for NOES sheets, namely cube $\{001\}\langle 100 \rangle$, rotated cube $\{001\}\langle 110 \rangle$, Goss $\{110\}\langle 001 \rangle$, and rotated Goss $\{110\}\langle 110 \rangle$ components, as well as α -, α^* -, γ -, η -, and λ -fibers⁵⁶.

$$\begin{aligned} \text{crystallographic texture X} &\sqsubseteq \\ &\exists \text{equality of. (grain population} \\ &\quad \sqcap \exists \text{has member. crystallite with X orientation} \quad (8) \\ &\quad \sqcap \forall \text{has member. crystallite with X orientation}) \end{aligned}$$

Axioms 6, 7, and 8 are applicable to any polycrystalline material in which crystallographic texture develops relative to a processing-induced reference frame, with material-specific crystallite orientation classes to be defined in the corresponding application-level ontology. The usage of these axioms for inferring macroscopic crystallographic texture is demonstrated in Section [Scenario 4: Inference of the macroscopic texture](#).

Fractions of texture components Macroscopic crystallographic texture is often quantified using fractions of texture components and fibers, determined by post-processing XRD or EBSD data to investigate the origin of anisotropy of functional properties⁷². To address CQ8, a design pattern for formally describing the fractions of specific texture components and fibers is shown in Figure 11, where a grain population with a specific crystallographic texture is part of the microstructure of a rolled metal sheet, and the fraction of these grains is expressed relative to the microstructure.

Usage scenarios

To demonstrate the practical application of the present semantic models and validate the formulated TBox against the defined CQs, an exemplary ABox is constructed using synthetic data consistent with typical NOES grades reported in the literature, covering chemical composition, manufacturing processes, the anisotropy of mechanical and magnetic properties, and fractions of crystallographic texture components. Three usage scenarios demonstrate SPARQL-based retrieval of explicit knowledge, corresponding to the manufacturing, microstructure and crystallographic texture, and functional property categories of the formulated CQs. A fourth scenario validates the inferential capabilities of the semantic models by applying logical reasoning to a real EBSD dataset⁷³ to infer macroscopic crystallographic texture from individual crystallite orientations. The queries and their results are provided in the GitHub repository of the ontology.

Scenario 1: Manufacturing process chain and process parameters To identify the manufacturing processes that a rolled metal sheet underwent, and the corresponding processing parameters, SPARQL SELECT queries based on CQ2 and CQ3 are executed against the exemplary ABox. The first query returns the complete manufacturing history of the NOES sheet as an ordered sequence of processing steps, expressed by asserting *bfo:precedes* relations between processes. The second query retrieves process attributes and their values for a given process whose class URI is provided as input.

Scenario 2: Microstructure and crystallographic texture As the functional properties of NOES are governed by its microstructure and crystallographic texture, querying these features is essential to unravel the PSP dependencies. Two SPARQL SELECT queries address CQ6 and CQ8, retrieving the average grain size of the material and the volume or area fractions of characteristic texture components, respectively. The texture component fractions retrieved by the CQ8-based query can be combined with an assessment of property anisotropy. An additional

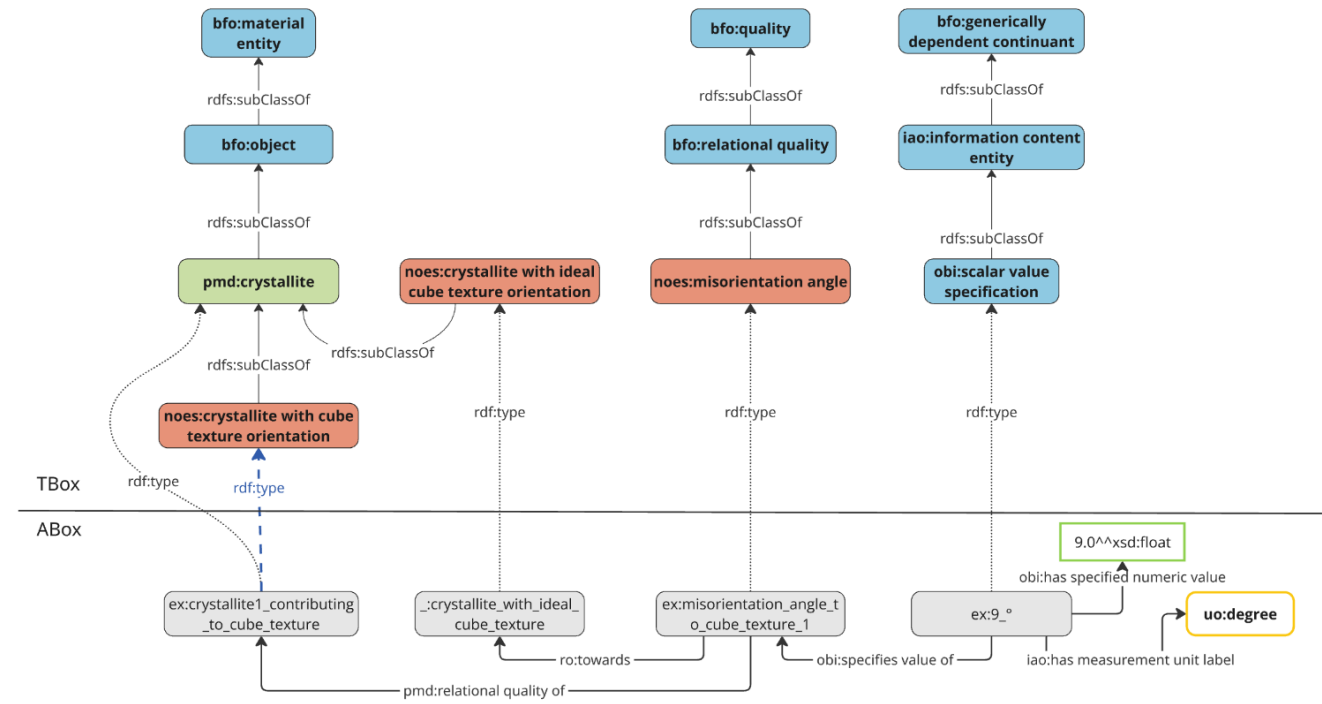


Figure 10. An exemplary inference of a crystallite with cube texture orientation (TBox/ABox view). The blue dashed line indicates a triple inferred via logical reasoning. A misorientation angle between the considered crystallite and the ideal crystallite is 9 degree, i.e., below the texture tolerance threshold. Consequently, `ex:crystallite1_contributing_to_cube_texture` is classified as **noes:crystallite with cube texture orientation**. The ideal crystallite `_:crystallite_with_ideal_cube_texture` is represented as a labeled blank node.

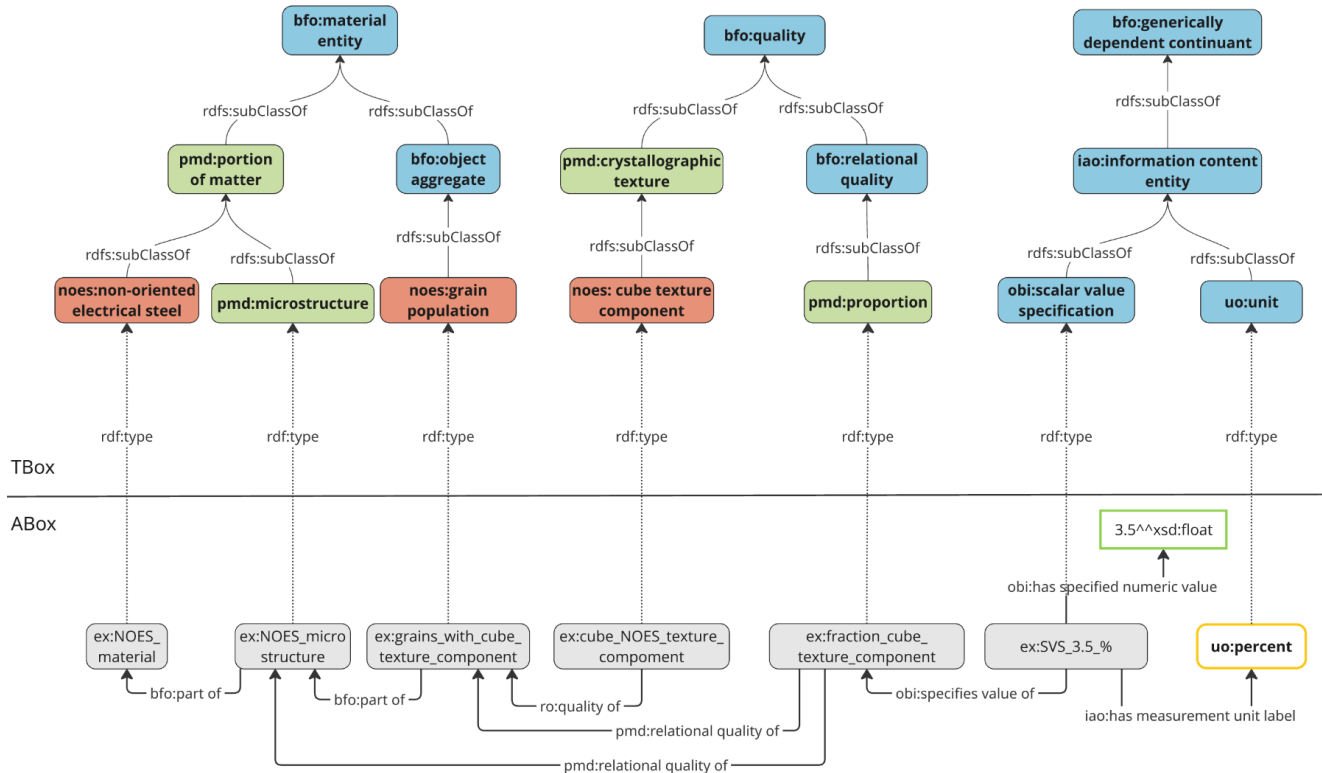


Figure 11. Design pattern for the semantic description of fractions of texture components and fibers (TBox/ABox view). A parthood relation is asserted between the material and its microstructure, and between the microstructure and the grain population with the cube texture component. The fraction of these grains is expressed as an instance of **pmd:proportion**, related to the grain population and microstructure via *pmd:relational quality of*.

SPARQL SELECT query retrieves the values of a user-specified property measured at different orientations relative to the RD, with

the property type provided as input via its class URI. The direction-specific property classes are inferred based on Axiom 4, without requiring explicit type assertions in the ABox.

Scenario 3: Functional properties and anisotropy CQ10 addresses the dependence of functional properties on the chemical composition of NOES. The corresponding SPARQL SELECT query takes a user-specified chemical element with its lower and upper boundary values as input and retrieves the mass percentage of the specified element in the alloy along with values of a user-specified functional property. Additionally, the query retrieves the most specific class from the taxonomy for every property individual, where direction-specific classes are inferred using Axiom 4.

CQ11, CQ12, and CQ13 address material performance under specified operating conditions and the interplay between mechanical and magnetic properties of NOES sheets, guiding domain experts in material selection for the specific application. A single SPARQL SELECT query jointly addresses these CQs. In the query, a user-specified mechanical property is selected, and its values are constrained by upper and lower bounds, addressing CQ13. The values of magnetic properties measured under alternating magnetic field conditions depend on the frequency f_{AC} and the target peak polarization J_{max} (or induction B_{max}), addressed by CQ11 and CQ12. The exemplary ABox only contains results of Epstein measurements performed at $f_{AC}=200$ Hz, with J_{max} values filtered in the query to not exceed 1.0 T. As NOES sheets are intended to exhibit isotropic properties within the RP, the query returns the averaged mechanical and magnetic property values under the specified conditions for each material in the ABox, enabling direct comparison of the interplay between these properties across materials. This is particularly relevant for high-torque or high-speed electric vehicle applications, where performance requirements differ⁷⁴.

Scenario 4: Inference of the macroscopic texture The present semantic models for the formal description of crystallographic texture enable automatic inference of the macroscopic texture from the orientations of individual crystallites. To demonstrate these inferential capabilities, the dataset⁷³ was used, which provides crystallite orientations of an NOES sheet in Bunge Euler angle format, along with the areas of individual grains in μm^2 , as obtained from EBSD measurements. The workflow of the inference is illustrated in Figure 12.

First, misorientation angles of all crystallites to every ideal texture component and fiber are calculated from the Euler angles using the orix Python package⁷⁵. A KG is populated using a SPARQL CONSTRUCT query asserting the misorientation angles (Axiom 7) and the areas of individual grains. To reduce reasoning efforts, only orientations of texture-relevant crystallites, i.e., those falling within the 15° misorientation tolerance, are included. The classes of crystallites with characteristic orientations are inferred based on Axiom 7 using the Konclude reasoner⁷⁶. As OWL 2 DL reasoning cannot create new named individuals, the instantiation of **noes:grain population** individuals and the assertion of *ro:has member* relations must be handled externally. These steps, along with the instantiation of **pmd:crystallographic texture** and the corresponding *ro:has quality* relation between the grain population and the texture (Axiom 8), are handled via a dedicated SPARQL CONSTRUCT query. Lastly, the area fractions of characteristic texture components are computed using a SPARQL SELECT query, and added to the KG via graph conjunction using the rdflib Python package⁷⁷.

Axioms 7 and 8 are validated by comparing the values of area fractions of texture components determined via OWL 2 DL + SPARQL workflow with the results calculated solely by orix through post-processing of the misorientation angles. As shown in Table 2, the area fractions of texture components and fibers are in agreement across all texture components. This comparison serves to validate the correctness of the introduced axioms rather than to propose a replacement for established texture analysis tools such as orix. Notably, the misorientation angles provided by orix serve as input to both approaches, with the key difference that the graph-based approach yields a formal, FAIR representation of individual grain orientations, macroscopic crystallographic texture,

and the relation between them within a single queryable KG. The constructed KG can be directly used for downstream graph-based approaches without requiring a semantic bridge between different texture representations. For example, the correlation between crystallographic texture and the anisotropy of functional properties can be formally investigated, or crack propagation in textured materials can be related to individual grain orientations.

Table 2. Validation of texture inference rules (OWL 2 DL + SPARQL) by comparison of area fractions of texture components given in % with orix

	orix	OWL 2 DL + SPARQL
Cube	1.98	1.98
Rotated Cube	2.30	2.30
Goss	2.08	2.08
Rotated Goss	0.00	0.00
α -fiber	14.63	14.63
γ -fiber	17.93	17.93
η -fiber	10.67	10.67
λ -fiber	15.20	15.20

Discussion

Capabilities of the present semantic models

The formalization of the manufacturing process chain using TQCs represents a pragmatic, application-agnostic approach to the semantic description of the evolution of material state across sequential processing steps. This modeling pattern is not specific to rolled metal sheets and is directly transferable to any material class whose properties evolve across a manufacturing process chain. A key advantage of this representation is the flexibility to designate material characteristics as time-invariant or time-variant, depending on the required modeling granularity and the phenomena of interest.

The semantic models for the formal description of property anisotropy, while motivated by the directional dependence of functional properties in NOES sheets, are largely application-agnostic. The anisotropy axiom (Axiom 4), grounded in the formal description of specimen orientation via relational qualities, is applicable to any material whose properties are investigated by varying the orientation of a specimen relative to some reference. Furthermore, the use of logical reasoning to automatically classify direction-specific property instances eliminates the need for manual annotation of measurement results, reducing the semantic burden on data providers and enabling systematic comparison of property magnitudes across orientations via SPARQL SELECT queries.

The **Usage scenarios** demonstrate that the formulated TBox successfully addresses the in-scope CQs across all three categories: manufacturing, microstructure and crystallographic texture, and functional properties. Beyond individual retrieval, CQs from different categories can be composed into queries that directly target PSP dependencies. Process-Structure dependencies become queryable by combining CQ2 with CQ6 and CQ7. As material states across the manufacturing chain are ordered via TQCs (Section **Temporally qualified continuants in the manufacturing process chain**), the evolution of microstructural features at each processing step can be retrieved without additional modeling effort. Extending the query with CQ3 further enables linking the process parameters associated with each step to changes in the microstructure, providing a basis for data-driven process optimization grounded in semantically enriched PSP data. Structure-Property dependencies can be investigated by querying for an average grain size (CQ6) and inclusion content, quantified as a volume fraction or number density (an extension of CQ7), together with functional property values (CQ10-CQ13). As performance requirements for NOES sheets vary with operating

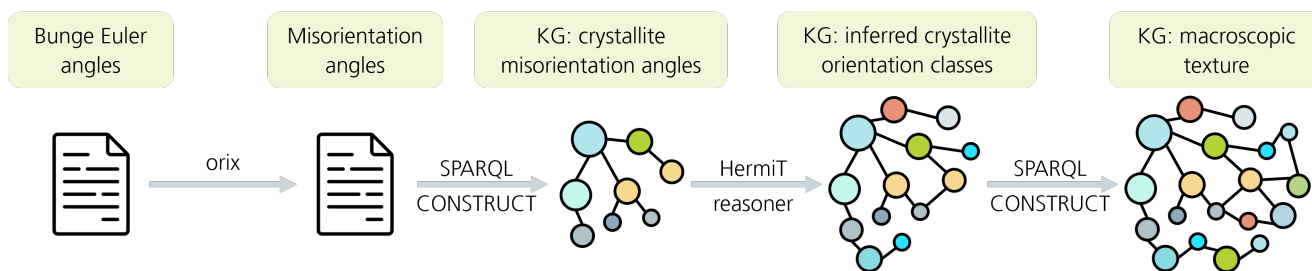


Figure 12. The workflow for the inference of the macroscopic crystallographic texture from an EBSD dataset containing crystallite orientations.

conditions⁷⁴, such combined querying supports the identification of microstructural features that either positively influence the target functional property or achieve a balance between magnetic and mechanical performance.

The present semantic models also provide a framework for detecting correlations between crystallographic texture and property anisotropy. By combining a query for texture component volume fractions (CQ8) with queries for functional properties (CQ11-CQ13), the influence of individual texture components on property anisotropy can be investigated. Notably, neither the anisotropic property class nor the texture component class needs to be explicitly asserted. The direction-specific property is inferred using the logical Axiom 4, where only the cutting direction of the specimen must be asserted. The crystallographic texture component or fiber is inferred using Axioms 7 and 8, where it is sufficient to assert the misorientation angles between crystallite orientations and the ideal texture component or fiber orientations.

Limitations of the present semantic models

Out-of-scope competency questions Addressing some of the CQs given in Table 1 is deferred to future versions of the present semantic models. For example, CQ4 requires a formal description of the cutting and coating processes for rolled metal sheets, which represent downstream manufacturing processes beyond the material-focused PSP scope of this work. CQ5 addresses the influence of the flatness deviation of a single sheet on the geometry and performance of a stator stack. Addressing these CQs requires bridging the material-level properties of an individual sheet and the component-level performance of a sheet stack. Cutting techniques induce local deformation of magnetic domains, resulting in distortion of the magnetic field and increased total losses of the stator^{78,79}. Flatness deviation introduces gaps between stacked sheets, uneven cutting edges create geometric irregularities at sheet boundaries, and defects in the coating layer reduce electrical insulation, all of which contribute to increased eddy current losses in a stator stack. As these effects accumulate across all sheets in the stack, it is not trivial to correlate performance at the material and component levels. Formally addressing this correlation requires a description of the coating materials and processes, the cutting parameters, induced local effects at cutting edges, and the geometry and functional properties of stator cores. Extending the present semantic models towards a component-level description of stator performance necessitates a dedicated application-level ontology, built upon the BFO-aligned semantic models developed in the present work.

CQ9 necessitates a dedicated formal model to describe microstructural features such as dislocations and shear bands. As these features are relevant to a broad range of metallic materials beyond rolled metal sheets, their rigorous formal description is better addressed by a dedicated, more general ontology for metallic microstructure rather than within the present use-case-specific scope. Lastly, CQ14 requires a semantic description of computational methods for material investigation to formally distinguish and compare experimentally measured and computationally derived property values. As this comparison is

relevant across all MSE domains, the dedicated semantic models are to be developed at the domain level, e.g., in future versions of PMDco 3.0.

Challenges associated with representing crystallographic texture in BFO Crystallographic texture describes the statistical distribution of grain orientations, expressed as a relation between the external reference frame of a sample and the internal reference frames of individual volume units. Bunge Euler angles statistically describe the orientations of crystallites, as quantified by techniques such as XRD, whereas axis-angle pairs or orientation matrices define the orientations of individual volume units, as obtained from EBSD measurements. The formal representation of these orientations within the BFO framework is non-trivial, as no prior work has formally defined reference frames or rotational transformations between these. For example, to infer texture $\{hkl\}\langle uvw \rangle$ notation of grain orientations from Bunge Euler angles would require complete formal definitions of the rotation axis, rotation direction, and the resulting axis position for each of the three successive rotations, along with the non-commutative composition of these transformations, all of which would require mathematical transformations beyond OWL 2 DL inferential capabilities. Similarly, determining whether the misorientation between a real and an ideal orientation falls within the 15° threshold requires a matrix operation between the two orientations, which OWL 2 DL cannot perform.

A further challenge concerns the formal definition of directionality for RD, TD, and ND. In the current version, these are implemented as subclasses of **bfo:fiat line**, a one-dimensional, immaterial entity that is inherently undirected, contradicting the directionality of the applied force in rolling. A fully directional definition would require an associated reference frame specifying a start and an end point. However, such a reference frame would naturally be anchored to a stationary spatial region of the rolling mill, whereas RD, TD, and ND persist as properties of the sheet after rolling and are spatially independent of the manufacturing equipment. Such persistence of characteristic directions in the material complicates a formal definition of directionality. A similar challenge is addressed in the Biological Spatial Ontology (BSPO)⁸⁰, which represents anatomical axes with persistent directionality by implicitly encoding direction in the class label rather than through an explicit formal definition, e.g., **bspo:left-right axis**. The present modeling of RD, TD, and ND follows a similar pragmatic approach. The modeling scope can be further extended by introducing additional resources, e.g., a class **noes:anti-rolling direction** and a corresponding object property **noes:anti-parallel to** to formally distinguish opposing directions along the same fiat line.

Scalability limitations of logical reasoning for inference of crystallographic texture Computational scalability presents a further practical limitation. The behavior of the Konclude reasoner⁷⁶ on various ABox sizes is shown in Table 3. The fully filtered ABox contained only triples of crystallites with at least one misorientation angle below the 15° threshold, and triples corresponding to misorientation angles above this threshold were removed; the semi-filtered ABox contained only relevant

crystallites, but all the misorientation angles were retained; no triple filtering was performed on the full ABox. The classification of crystallites based on Axiom 7 successfully finished only on the fully filtered ABox. Notably, the triples *pmc:has relational quality* and *ro:towards* were stripped from the reasoned ABox in both semi-filtered and full KGs, justifying the failure of crystallite classification. To investigate this unstable reasoning behavior, the classification was performed on semi-filtered KGs of several sizes with randomly selected crystallites. The classification finished successfully for all ABox sizes with fewer than 583 crystallites (33239 triples) but failed for larger KGs due to the stripping of triples. Reasoning over semi-filtered and full ABox using the HermiT reasoner⁷⁰ was terminated after exceeding the time limit of 2 hours. These results motivated the filtering of the ABox in [Scenario 4: Inference of the macroscopic texture](#). While this filtering significantly reduces reasoning efforts, it introduces an additional pre-processing step that partially mitigates the need for logical reasoning using Axiom 7. Alternatively, the filtered orientations could be asserted directly as instances of the corresponding crystallite with specific texture classes via SPARQL CONSTRUCT. The value of maintaining the reasoning step lies in the formal semantics, as the axiom-based classification is derived from the ontological definition of texture components, ensuring that the resulting KG is semantically consistent and extensible to new texture components without modifying the pipeline. A further reasoning scalability concern arises from using a SPARQL CONSTRUCT query to assert texture component or fiber subclasses based on Axiom 8. The explicit assertion of texture component or fiber subclasses could alternatively be replaced by inference by reformulating Axiom 8 as a necessary and sufficient condition and asserting the exhaustive list of crystallites in a grain population. However, this approach requires a second DL reasoning pass, which is more computationally expensive than the SPARQL CONSTRUCT approach adopted here.

Conclusions and outlook

In this work, semantic models for the formal description of PSP dependencies in rolled metal sheets were introduced, covering the manufacturing process chain, microstructural features, crystallographic texture, and the anisotropy of functional properties. In contrast to existing steel manufacturing ontologies, which primarily address machinery control or data-processing workflows, the present semantic models focus exclusively on the formal description of PSP dependencies. The models are aligned with the BFO via PMDco 3.0, thereby establishing the semantic interoperability required to conform with the FAIR data principles. This is an important prerequisite for establishing a shared data space where knowledge from heterogeneous sources can be integrated throughout the entire PSP chain. The formal symbolic representation of the high-dimensional PSP space provides a necessary foundation for data-driven approaches to multi-objective materials optimization.

While the present semantic models were validated for the NOES sheets use case, the formulated logical axioms are neither constrained to the specific material class nor the rolling process chain. In fact, the patterns for the semantic description of texture can be similarly applied to other crystallographic texture-inducing forming processes, such as extrusion, forging, deep drawing, 3D printing processes, and epitaxial thin film growth. The TBox can be extended to reflect additional processing steps, microstructural features, or functional properties relevant to other material classes, without requiring modification of the underlying logical axioms. A direction for future work is therefore to extend present semantic models towards a more general semantic description of materials exhibiting anisotropy of properties resulting from the manufacturing process chain and provide a dedicated ontology for this purpose.

The validation against the formulated CQs demonstrated that the present semantic models address individual aspects of the PSP space, and combining CQs across categories enables the formal description of PSP dependencies. The inferential capabilities of the models, e.g., the automatic classification of crystallographic texture and direction-dependent functional properties, support the unraveling of PSP dependencies while keeping the asserted ABox comparatively simple. Post-processing data represented in KGs, particularly using methods that account for symbolic knowledge representation, can facilitate the inference of implicit knowledge in this domain, thereby accelerating materials development.

Future development of the present semantic models will follow several directions. First, the CQs identified as out of scope in the current version define an immediate development roadmap. Second, extending the scope beyond the performance of the rolled metal sheet itself to the performance of components manufactured from it is planned, as component-level performance is the most relevant aspect from an industrial perspective. Third, the challenges related to the formal description of reference frames and rotational transformations in BFO, the representation of misorientation tolerances within OWL 2 DL, and the extension of texture axioms to lower-symmetry lattice systems define the future work at the intersection of ontology engineering and crystallography.

Data Availability

The ontology presented in this study, SPARQL queries based on the formulated competency questions, the synthetic ABox dataset, and a Python script for the inference of macroscopic texture are openly available. They can be accessed and obtained from the following GitHub repository and URLs:

- [NOES Onto: Non-oriented Electrical Steel Ontology](#)
- [Reports on quality assessment of NOES-Onto](#)
- [SPARQL queries](#)
- [Synthetic ABox](#)
- [All the files related to the inference of macroscopic crystallographic texture](#)

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Declaration of conflicting interests

Author Kamilla Zaripova was employed by Schaeffler Technologies AG & Co. KG. Authors Peter Gebauer and Andreas W. Müller are employees of Schaeffler Technologies AG & Co. KG by the time of writing.

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Consent to participate

All participants in user interviews provided implicit informed consent by accepting the meeting invitation, which included a brief description of the purpose of the interview.

Author Contributions

Kamilla Zaripova: conceptualization (lead); investigation (lead), data curation (lead); formal analysis (lead); methodology (lead);

Table 3. Comparison of reasoning behavior using Konclude across different ABox sizes for the crystallite classification using Axiom 7

ABox variant	ABox triples	crystallite-angle pairs	CPU time (s)	Peak RSS (MB)	Successful run
Fully filtered	12599	1644	3.10	700	Yes
Semi-filtered	61739	8664	1.06	231	No
Full	130540	18320	2.07	415	No

software (lead); validation (lead); visualization (lead); writing — original draft (lead). **Ali Riza Durmaz:** conceptualization (equal); funding acquisition (lead); supervision (equal); writing — review and editing (equal); software (supporting). **Philipp von Hartrott:** conceptualization (equal); supervision (supporting); writing — review and editing (supporting). **Akhil Thomas:** supervision (supporting); writing — review and editing (supporting). **Andreas W. Müller:** investigation (supporting); validation (supporting); writing — review and editing (supporting). **Peter Gebauer:** validation (supporting); writing — review and editing (supporting). **Harald Sack:** validation (supporting); writing — review and editing (supporting). **Chris Eberl:** conceptualization (equal); supervision (equal); writing — review and editing (supporting).

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