OntOMat - Towards an Ontology-based Integration of Manufacturing and Simulation Processes for Fiber-reinforced Materials

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Abstract

The rapidly expanding market for composite materials, driven by applications in automotive, aerospace, and renewable energy, requires a comprehensive framework to describe fiber-reinforced materials. Although versatile, these materials lack standardized data representation, hindering cross-scale integration from material characterization to manufacturing. The OntOMat project aims to bridge this gap by developing a novel ontological framework grounded in FAIR data principles. Through ontology engineering, it enables the collection, linkage, and analysis of data across various processes, focusing on fiber-reinforced polymers. This approach allows for the optimization of material microstructures for enhanced stability and recyclability.

This paper describes the OntOMat ontology development process and its result, highlighting its novel classification techniques and the integration of the IEC 62474:2018 standard. In particular, it introduces an innovative semantic representation of the VDI 3682 visual process language, paving the way for detailed multiscale simulations. The current ontology, though promising, has limitations, such as incomplete support for parallel processes and coarsely modeled technical resources. Ongoing work includes refining the ontology to address these constraints, enhancing data injection tools, integrating existing modeling tools, and developing a GenAI-based copilot for intelligent interaction with the knowledge base.

1. Introduction

The market for composite materials is growing at double digit percentages annually [1], as composite materials allow lightweight applications in the construction of automobile, train, ship, and aircraft, as well as renewable energy, such as wind turbine blades. Due to the non-standardized nature of composites and in particular fiber-reinforced materials, thousands of possible material systems need to be described. Currently, a harmonized description including cross-scale relationships between material, process, and component is not available for them. In addition, there is insufficient data integrity with respect to material characterization, simulation, and manufacturing processes. The implementation of FAIR data principles [2] and semantic technologies, such as ontologies, should allow us to describe these material systems and represent complex cross-scale relationships. This is intended to open up previously unusable potential for data-driven material development and process optimization, as well as the establishment of material cycles.

The main goal of the OntOMat project is to develop a novel ontological framework that allows the implementation of FAIR data principles using ontology engineering. This should allow us to collect, link, and analyze data arising from material data sheets, but also from characterization, production, and simulation processes which are collected for a variety of material systems. In terms of material systems, the focus is on fiber-reinforced polymers. The linking of data and parameter arising from these

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processes should then allow us to compare and optimize a material's microstructure for operational stability and recyclability. The scope can be directly derived from the project goal and includes the creation of an ontology for (a) fiber-reinforced materials and their characteristics, (b) the manufacturing and characterization processes of these materials, and (c) the simulation processes to determine certain characteristics or behavior. In this paper, we first present our ontology development methodology (Section 3), then give the details of the OntOMat ontology (Section 4) and discuss limitations and future work (Section 5).

2. Related Work

For an extensive survey of ontologies in materials science and engineering, we refer to [3] and give more details on the relevant top- and midlevel ontologies in Section 3. From the domain-level ontologies presented in [3], the EMMO General Process Ontology (GPO), the Semantic Materials, Manufacturing and Design[1] (SEMMD) ontology, the Additive Manufacturing Ontology (AMONTOLOGY), Ontology for Simulation, Modelling, and Optimization (OSMO), Dislocation Simulation and Model Ontology (DSIM), Atomistic Simulation Methods Ontology (ASMO), Metadata4Ing Ontology (M4I), and Material properties ontology (MAT) covers the same domains as our work. Since the OntOMat project is part of *Platform MaterialDigital*[2] that provides a top-level ontology with the BFO[4] and a mid-level ontology with the PMD Core Ontology[3] (PMDCo), we focus only on ontologies that align with the BFO or PMDCo, since alignments with other top-level ontologies are beyond the scope of this work. The SEMMD ontology is concerned with the same focus and is already BFO aligned, but any documentation regarding its use is missing. Ontologies that describe either composite materials or VDI/VDE 3682 Formal Process Language (VDI 3682 language) are harder to find. Polymer membrane research and related laboratory experiments are described in the PolyMat ontology [5], but the ontology does not seem expressive enough to capture, e.g., complex simulations. An initial ontology for the VDI 3682 language was introduced in the work of [6], which we considered in our ontology design. However, the work of [6] missed certain design elements, such as process decompositions and alignment with any top-level ontology.

3. Ontology Development

We apply the "Simple Knowledge Engineering Methodology" of [7] to develop our ontology. It offers good guidelines for an agile modeling process. For brevity, we recapture the main steps introduced by the authors of [7] and give more details in the following subsections:

1. Domain and scope of the ontology that includes competency questions for narrowing the scope;
2. Reuse of existing ontologies that includes an alignment with mid- or top-level ontologies;
3. Collect important terms and define classes and their hierarchies in the ontology, which can be addressed by top-down, bottom-up or combined approach;
4. Define properties of classes including "slots" such as cardinality and domain/range;
5. Define instances, which includes generic instances that should be available for every user, but also includes illustrating examples.

Note that above steps are a non-linear process of incremental interactions (in particular steps 3. to 5.). Hence, the terms for a specific topic are collected by domain experts, mainly material scientists but also simulation engineers, stored in an intermediate source, which then builds the base to define classes and properties. The authors then present the results including class and property hierarchies to the aforementioned domain experts for evaluation.

[1]https://github.com/cpauloh/semmd
[2]https://www.materialdigital.de/
[3]https://materialdigital.github.io/core-ontology/index-de.html

3.1. Competency Questions

The first step of [7] relates to the collection of more than 50 competency questions with the experts of the OntOMat partners. They are categorized by “material testing/characterization”, “manufacturing process and equipment”, “physical product traceability”, “material consumption”, “product life cycle and design”, and “material testing/characterization”. In the following, we present a list of exemplary competency questions (CQs) and expected exemplary answers:

Competency question	Expected answer
Which characterization methods can be used for a certain material property?	Certain material properties can be quantified by specific characterization techniques. A CT scan can be used to quantify, e.g., the fiber volume content of a composite material.
What characterization methods can be applied within a manufacturing process?	The existing processes show that digital holography is an in-situ process operator.
What parameters are required to run a specific simulation?	Specified material information including the material properties and values as well as defined geometry to be modeled along with the physics to be analyzed, e.g., structural mechanics, are needed. In addition, the loads and boundary conditions need to be defined and the geometry needs to be discretized in order to numericial solve the differential equation.
How can data from the characterization be implemented into the simulation model?	Test results can be reduced to effective parameters, e.g., the modulus of elasticity, which is then used in a suitable numerical model.
What contributes to product durability?	Durability means change of material properties values over time. Durability therefore depends on the operational conditions applied as well as the impact on specific material properties.
Which simulations can be used for a certain material system?	There is no clear relation between material class and simulation technique, but there is a relation between simulation domain and physics to be studied for a certain material class.
What characterization data are needed for a specific material model or simulation?	The material model requires certain parameters to be defined. The parameter values can be retrieved from specific characterization techniques that quantify material property values.
What substances are contained in a specific material class?	A fiber-reinforced epoxy resin has epoxy resin (61788-97-4) as the matrix and carbon fibers (7782-42-5) as the reinforcement.
What are the relevant material properties for a specific material class?	Test results can be reduced to effective parameters, e.g., the modulus of elasticity, which is then used in a suitable numerical model.
Show the impact of recycled material content on material properties and manufacturing processes?	Compared to virgin materials, the property values can significantly deviate for materials containing recycled material content, even if the material composition is kept constant.

Based on the competency questions, we can derive important concepts, including material properties and compositions, as well as a model for simulation, manufacturing, and characterization processes, including process parameters and results, which play a crucial role for answering the CQs. We also provide the full list of CQs in our project’s Gitlab repository.

3.2. Ontology Reuse

The second step of [7] is the alignment with a mid-/top-level ontology. Ontology reuse is along a pyramid, where the top-level has the highest abstraction level and are usually called upper ontologies. Examples are Basic Formal Ontology (BFO) [4] and Industrial Data Ontology (IDO) [8] with a focus on industrial data. Below are mid-level ontologies that describe a specific technical domain such as Quantities, Units, Dimensions and Data Types Ontologies (QUDT)[4] or PROV Ontology (PROV-O) [9] which are often orthogonal to upper ontologies. Domain ontologies, such as Elementary Multiperspective Material Ontology (EMMO) [10][5], describe a specific scientific or industrial domain, where the OntOMat ontology would be one particular domain.

As the OntOMat project is situated at the intersection of industrial data/processes and material science, the IDO ontology is a natural starting point for modeling, since simulation and manufacturing processes are an important scope of the vocabulary. Another option would have been the PMDCo 1.0 ontology based on PROV-O, which provides some useful top-level concepts, such as Activity, but it lacks the coverage and standards compliance to known top-level ontologies such as BFO. With the publication of the PMDCo 3.0 ontology that is based on the BFO the coverage and standards compliance is given, and in the discussion we will outline the path towards a tighter integration with the PDMCore 3.0.

3.3. Conceptualization

For the OntOMat ontology in most cases, the IDO classes and properties build the highest level of class hierarchies, whereby the classes `lis:PhysicalArtefact`, `lis:PhysicalObject`, `lis:Quality`, `lis:Activity`, and `lis:InformationObject` are our anchor points. An important characteristic of IDO modeling is the distinction of any object (besides information) between `lis:Specified`, i.e., any abstract representation of an object such as a definition or simulation model, and `lis:Actual`, i.e., objects that exist or existed at one point.

The third step of [7] is the collection of important terms that lead to classes and related properties. Initially, we manually collected terms based on standards and guidelines with the support of domain experts. For example, experts suggested a material classification according to the IEC 62474 standard [11] and a formalized process description (FPD) according to the VDI/VDE 3682 guidelines [12] as important sources. For material qualities, the domain experts suggested a list of 150 relevant qualities based on literature research, which we extended with units and symbolic representations. Material classes and qualities were collected as term lists and taxonomies in newly created spreadsheets, while processes, states, and operators of the FPD were directly extracted from the text-based guidelines. With the fourth step, we bring all the pieces together, where we created an initial version of the ontology formulated in OWL 2 DL[6]. We decided on a modular approach that creates a separation between terms related to *material products*, to *material and properties classes*, and to *processes* that include simulations. Each module was validated by our domain experts for content-related correctness, which led to several rounds of improvements. The ontology described in the next section represents the result after the completion of the fourth step.

4. The OntOMat Ontology

The OntOMat ontology (OMO) is conceptually split into three tiers, where the top level is currently IDO, the middle level is a handcrafted structure with the support of domain expert, and the lowest level is automatically generated based on two industry standards concerning material classes and process descriptions. An important part are material classes and material qualities, i.e., material properties, which are then used to define material products based on these material classes. Another important

[4]https://www.qudt.org/
[5]EMMO also introduces its own top-level and mid-level vocabulary, rather than re-using existing ones.
[6]https://www.w3.org/TR/owl2-overview/

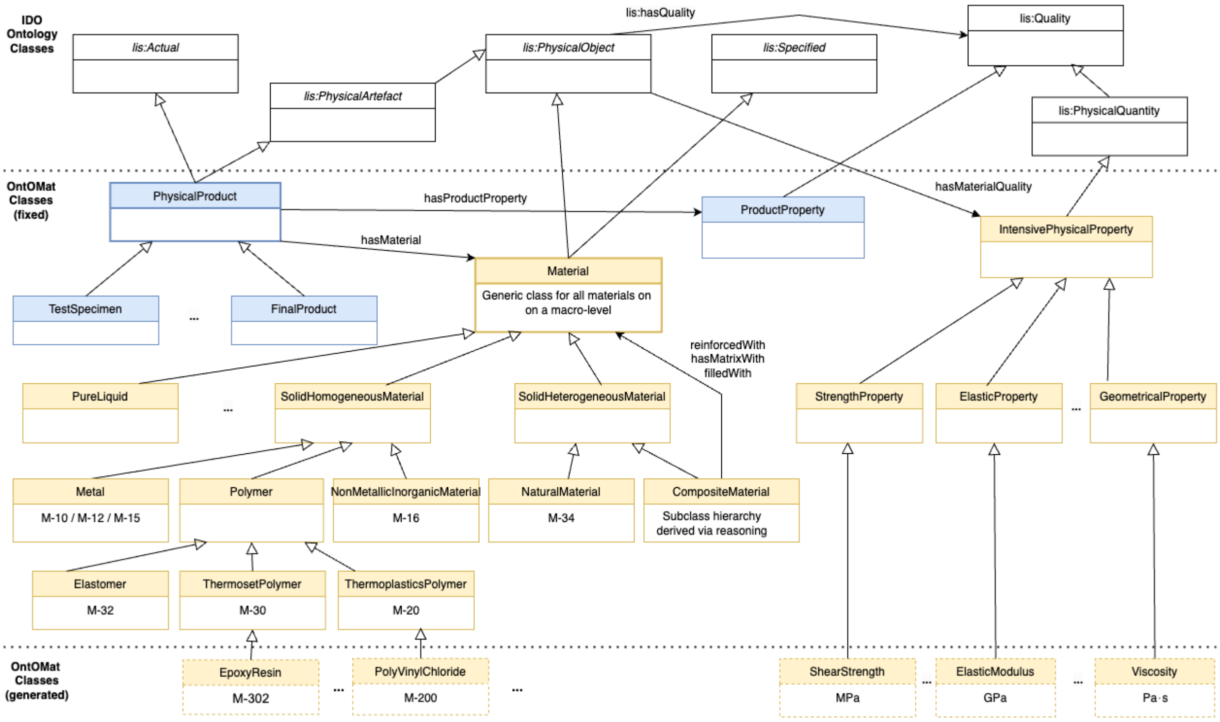


Figure 1: Overview of the three tiers of the OntOMat ontology; a partial rendering of the ontology is shown.

part describes the characterization, manufacturing, and simulation processes from an "a posterior" perspective, thus the process path (e.g., based on observations stored in logs) of the respective process is captured, and (currently) not the process plan modeled "a priori". Figure 1 shows the three tiers, where the color of the box represents thematic modularization, the white arrows represent the subclass relations, and the black arrows define the domain / range of object properties. The ontology is published on the MaterialDigital Github repository under https://github.com/materialdigital/ontomat-ontology.

4.1. Physical Products, Material Classes, and their Property Classes

With OMO, we introduce a duality between "real" physical products represented by `PhysicalProduct` and abstract material classes simply called `Material`. A physical product is made of one or more materials represented by material classes and is connected by the `hasMaterial` object property to a physical product.[7] Measurable material properties are connected by `hasMaterialQuality` with the domain `lis:PhysicalObject` (thus any physical object can have material properties) and the range of `IntensivePhysicalProperty` and subclasses that define types of material properties. Specific properties can be "real" properties of a physical product, which are measured as values of the designated specimen, or "abstract" properties of the material obtained from a product datasheet / publications. This duality allows us to manage the known material properties for material classes and their values only once and reuse them for every specimen. For example, the density of the material (class) gold is approximately 19.3 g/cm^3, but the density of a specific gold bullion is measured as 19.2 g/cm^3 due to some contamination.

The hierarchy of material classes starts with the `Material` class with a fixed set of subclasses derived from the IEC 62474:2018 standard taxonomy. The left nodes in the IEC taxonomy are automatically generated based on the standard spreadsheet shown in Figure 2a.[8] However, the IEC 62474:2018 standard misses some concepts to describe fiber-reinforced materials:

[7] `hasMaterial` is a subproperty of IDO's `lis:hasMaterialPart`, which has the domain `lis:Compound`. We extended the domain to include `Material`, since the ontology should also cover composites.
[8] https://std.iec.ch/iec62474/iec62474.nsf/Index?open&q=161936

Cat1	Cat2	SuperClass	ID	ClassName	CASNumber	ChEBI	Definition
1 Inorg	**M-10 Steels**	**SteelOrFerrousM**	**M-100**	**Stainless steel**	**12597-68-1**	CHEBI:18248	A group of corros
1 Inorg	M-10 Steels	SteelOrFerrousMa	M-101	Cast or sintered iron	11097-15-7	CHEBI:18248	irons that have be
1 Inorg	M-10 Steels and ferrous materi		M-119	Other ferrous alloys, non-stainless steels			iron and any alloy
1 Inorg	**M-12 Non-fe**	**NonFerrousMeta**	**M-120**	**Aluminium or aluminium alloy**	**7429-90-5**	CHEBI:28984	Aluminium and a
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-121	Copper or copper alloy	7440-50-8	CHEBI:28694	Copper and any
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-122	Magnesium or magnesium alloy	7439-95-4	CHEBI:25107	Magnesium and
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-123	Nickel or nickel alloy	7440-02-0	CHEBI:28112	Nickel and any a
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-124	Zinc or zinc alloy	7440-66-6	CHEBI:27363	Zinc and any allo
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-125	Lead or lead alloy	7439-92-1	CHEBI:25016	Lead, and its allo
1 Inorg	M-12 Non-fe	NonFerrousMetal	M-126	Tin or tin alloy	7440-31-5	CHEBI:27007	Tin, and its alloys
1 Inorg	M-12 Non-ferrous metals and a		M-149	Other non-ferrous metals and alloys			Other non-ferrous
1 Inorg	**M-15 Precio**	**PreciousMetal**	**M-150**	**Gold**	**7440-57-5**	CHEBI:29287	Gold, and its allo
1 Inorg	M-15 Precio	PreciousMetal	M-151	Platinum	7440-06-4	CHEBI:33364	Platinum, and its
1 Inorg	M-15 Precio	PreciousMetal	M-152	Palladium	7440-05-3	CHEBI:33363	Palladium, and it
1 Inorg	M-15 Precio	PreciousMetal	O-153	Silver	7440-22-4	CHEBI:30512	Silver, and its allo
1 Inorg	M-15 Precious metals		M-159	Other precious metals			Other precious m
1 Inorg	**M-16 Non-m**	**NonMetallicInorg**	**M-160**	**Ceramics**			An inorganic, nor
1 Inorg	M-16 Non-m	NonMetallicInorga	M-161	Glass	308066-74-2	CHEBI:131189	An inorganic, nor
1 Inorg	M-16 Non-m	NonMetallicInorga	O-162	Graphite	7782-42-5		An inorganic, nor
1 Inorg	M-19 Other inorganics		M-199	Other inorganic materials			Inorganic materia
2 Orga	**M-20 Unfille**	**ThermoplasticsP**	**M-200**	**PolyVinylChloride (PVC)**	**9002-86-2**	CHEBI:53243	A thermoplastic r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-201	PolyEthylene (PE)	9002-88-4	CHEBI:53227	Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-202	PolyPropylene (PP)	9003-07-0	CHEBI:53550	Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-203	PolyStyrene (PS)	9003-53-6	CHEBI:53276	Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-204	PolyCarbonate (PC)	25766-59-0	CHEBI:53201	Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-205	PolyOxyMethylene (POM)	9002-81-7	CHEBI:53421	Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-206	AcrylonitrileButadieneStyrene (ABS)	9003-56-9		Resin materials r
2 Orga	M-20 Unfille	ThermoplasticsPc	M-207	StyreneAcryloNitrile (SAN)	9003-54-7		Styrene Acrylonit
2 Orga	M-20 Unfille	ThermoplasticsPc	M-208	PolyAmide (PA)	63428-83-1	CHEBI:53224	Resin materials r

(a) Material classes

property super class	property class	property sub class	QUDT unit
Mechanical Physical Property	density		unit:KiloGM-PER-M3
Mechanical Physical Property	nominal weight		unit:GM-PER-M2
Geometrical Property	surface roughness		unit:MicroM
Geometrical Property	viscosity		unit:PA-SEC
Geometrical Property	dynamic viscosity		unit:PA-SEC
Geometrical Property	kinematic viscosity		unit:M2-PER-SEC
Thermal Physical Property	glass transition temperature		unit:K
Thermal Physical Property	water absorption		unit:PERCENT
Optical Property	refractive index		unit:UNITLESS
Optical Property	transmission coefficient		unit:UNITLESS
Optical Property	absobption coefficient		unit:UNITLESS
Optical Property	reflexion coefficient		unit:UNITLESS
Thermal Physical Property	melting point		unit:K
Thermal Physical Property	heat deflection temperature		unit:K
Thermal Physical Property	thermal conductivity		unit:W-PER-MK
Thermal Physical Property	heat transfer coefficient		unit:W-PER-M2-K
Thermal Physical Property	thermal expansion tensor coefficients	thermal expansion coefficient in x1	unit:PPM-PER-K
Thermal Physical Property		thermal expansion coefficient in x2	unit:PPM-PER-K
Thermal Physical Property		thermal expansion coefficient in x3	unit:PPM-PER-K
Thermal Physical Property	specific heat capacity		unit:J-PER_KiloGM-K
Elastic Property	symmetry class		unit:UNITLESS
Elastic Property	elastic modulus	elastic modulus E1	unit:GigaPA
Elastic Property		elastic modulus E2	unit:GigaPA
Elastic Property		elastic modulus E3	unit:GigaPA

(b) Material properties

Figure 2: Input spreadsheets of the IEC 62474:2018 standard.

- Classes representing fiber-reinforced composite materials are missing, only filled composites are mentioned;
- Only one class for gases and liquids is defined, whereby a clear separation between mixtures and pure gases (similarly for liquids) is missing;
- Thermosetting polymers, such as melamine formaldehyde (MF) and vinyl ester (VE) are not considered;
- The CAS registry number is missing, which is used to identify the most prominent chemical substance in a material.

With the support of our domain experts, we extended and refined the IEC 62474:2018 taxonomy, thus introducing the paired classes for gas (pure / mixture), liquids (pure / mixture) and solid materials (homogeneous / heterogeneous), as well as dropping all unspecified classes such as "other unfilled thermoplastics", which are covered by their superclasses. For example, we introduced the new classes `SolidHomogeneousMaterial` and `SolidHeterogeneousMaterial`, where from the latter we derived the subclass `CompositeMaterial`. This subclass is central to OMO and acts as the domain for the following object properties that define possible composite structures:

- `hasMatrixWith` denotes the matrix material, e.g., epoxy resin;
- `reinforcedWith` denotes the material that is used for reinforcement, e.g., fibers;
- `filledWith` denotes the material that is used as a a filler, e.g., air.

Note that for any of the above properties, we also added the transitive closure using a transitive property, since a material structure can have several levels of nesting. For example, we added the property `hasMatrixWithTransitive` for the `hasMatrixWith`. Similarly to the material class hierarchy, our experts conducted an extensive literature analysis to collect suitable property classes that were recorded in a reference spreadsheet. The spreadsheet defines the QUDT unit, a commonly used symbol, including aligned index usages, e.g., E_1, with respect to direction and symmetry class, e.g., isotropic. An excerpt of the reference spreadsheet is given in Figure 2b and again the respective subclasses such as `ElasticModulusE1` for "elastic modulus E1" are generated and aligned to the mid-tier, e.g., `ElasticProperty`, automatically.

4.2. Composite Material Classification

An objective of the OntOMat project is to provide an automatic classification of composite materials according to the structure of these materials. As shown in Figure 3, the classification of composite materials resembles the overlap of two hierarchies starting with `CompositeMaterial`, namely a matrix-based hierarchy (starting with `MatrixBasedCompositeMaterial`) and a reinforcement-based hierarchy starting with `ReinforcedCompositeMaterial`. Both hierarchies are joined again on the leaves, where the outcomes of the classification are added. For example, the leave class `FiberReinforcedEpoxyResin` is sub-class of `PolymerMatrixCompositeMaterial` and also of `FiberCompositeMaterial`. Having a wide range of possible materials that can act as a matrix (examples of suitable polymer classes are shown in Figure 2a) and act as reinforcements or fillings (such as `Carbon`), we introduced a classification system based on equivalence axioms. Our intuition is the following; on left-hand side of the equivalence is the class for the material system, for instance `FiberReinforcedEpoxyResin`, and on the right-hand side is an intersection of `CompositeMaterial`, a existential restriction on `hasMatrixWithTransitive`, in this case, `EpoxyResin`, and another existential restriction on `reinforcedWithTransitive` on `Material`. The generic `Material` class is used, since any material class could act as a reinforcement. The resulting equivalence axiom: $\texttt{FiberReinforcedEpoxyResin} \equiv (\texttt{CompositeMaterial} \sqcap \exists\texttt{hasMatrixWith.EpoxyResin} \sqcap \exists\texttt{reinforcedWith.Material})$, with $Tra(\texttt{hasMatrixWith})$ and $Tra(\texttt{reinforcedWith})$ is written in RDF 1.1 Turtle[9] notation as:

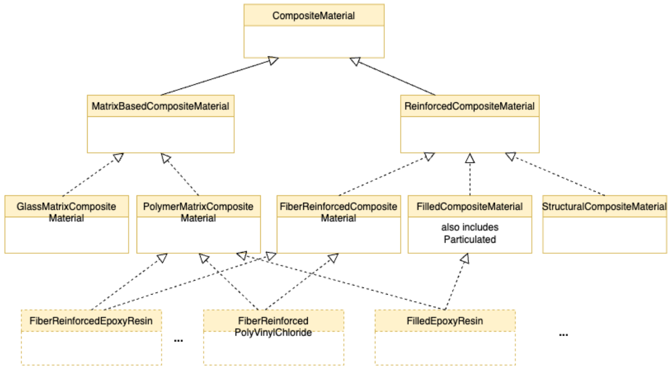


Figure 3: Partial rendering of the composite material classification.

```
ontomat:FiberReinforcedEpoxyResin owl:equivalentClass
    [ owl:intersectionOf (
        ontomat:CompositeMaterial
        [ rdf:type owl:Restriction ;
         owl:onProperty ontomat:hasMatrixWithTransitive ;
         owl:someValuesFrom ontomat:EpoxyResin
        ]
        [ rdf:type owl:Restriction ;
         owl:onProperty ontomat:reinforcedWithTransitive ;
         owl:someValuesFrom ontomat:Material
        ]
      ) ;
      rdf:type owl:Class
    ] ;
    dcterms:identifier "O-402" ;
    rdfs:label "Fiber-reinforced EpoxyResin (EP)" .
```

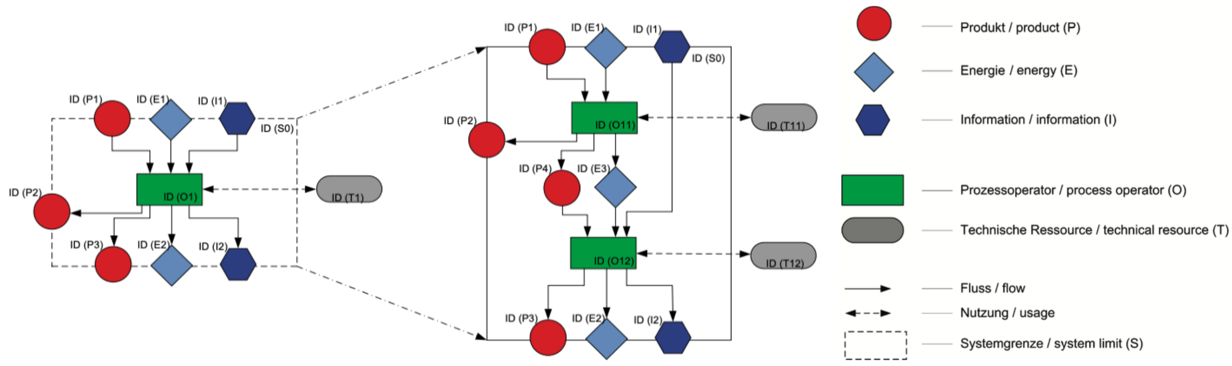
Listing 1: Example of an equivalence axiom with the OMO prefix `ontomat:`.

Taking the axiom from the listing above, `reinforcedWithTransitive` is replaced with `filledWithTransitive` to define filled composite material classes. The `Material` class could be replaced with `Carbon` to define more specialized systems such as `CarbonFiberReinforcedEpoxyResin`. Note that these axioms are automatically generated based on the spreadsheets shown in Figure 2a, where the "ClassName" column is parsed to extract the type of reinforcement and the matrix class.

4.3. VDI/VDE 3682 Formal Process Language

Despite several standards that are used to model processes, e.g., business process modeling and notation (BPMN),[10] no language captures all the aspects of technical processes that occur in engineering / industry applications, including their digital representation. The authors of the VDI/VDE 3682 Formal Process Language (VDI 3682 language) outline the following aspects that should be captured by a process language [12] used in engineering / industry applications:

[9]https://www.w3.org/TR/turtle/
[10]https://www.omg.org/spec/BPMN/2.0.2/



(a) An single process step and its decomposition (b) The eight graphical symbols

Figure 4: Overview of the VDI/VDE 3682 Formal Process Language.

- Modeling the life cycle of a technical systems, including its digital representation (usually called the digital twin);
- Applicable to all kinds of processes including technical / non-technical, continuous / batch processes in all fields of technical applications;
- Simple, neutral regarding the industry, and easily understandable;
- Containing all information necessary for engineering and normal operation based on modern IT tooling and methods;

The resulting VDI 3682 language is a visual language based on a predefined set of eight symbols (shown in Figure 4b) that include three *states*, a *system limit* (dashed frame), a *process operator* (green rectangle) and a *technical resource* (gray rectangle). The three kinds of states are *product* (red circle), *energy* (blue, rhombus), *information* (blue hexagon), which act as input and output of a process operator and are required to evaluate the operator. As shown in Figure 4a left, a process flow is always an alteration between states and process operators with reference to the technical resources used in that operator. In addition, the modeler has the choice to define parallel (the default) or alternatively running (similar to an XOR condition) process flows. A powerful feature of the VDI 3682 language is the ability to decompose a process operator into a new subprocess (shown in Figure 4a right), thus introducing modularity similar to functions in programming languages. The VDI 3682 guideline also introduces an UML-based data model and XML-based rendering of the visual language. We believe that the UML-based data model is a helpful sketch but is ambiguous regarding its serialization. In the second part of the guideline, the authors introduced an XML-based representation, which is sufficient for simple processes. However, this representation is underspecified and does not capture the full complexity of VDI 3682 process flows, for example, cyclic flows or subprocesses. Similarly to the authors of [6], we suggest that an ontology-based representation for the VDI 3682 symbols and workflows, as well as an RDF-based representation of (executed) workflows, are the most promising methods to capture it. Furthermore, material states can be defined more fine-grained by material classes, and similarly information states can be modeled by document and process parameter classes.

The ontology represented by [6] does not reuse any top-level ontology. Thus, we anchor our representation of the VDI 3682 language in IDO, where processes and operators are subclasses of `lis:Activity`, information states are directly mapped to `lis:InformationObject`, and production assets are subclasses of `lis:PhysicalArtefact`. As shown in Figure 5, the class `VDIProcess` is directly derived and includes subclasses such as `ManufacturingProcess` and `SimulationProcess`. Similarly the class `VDIProcessOperator` is directly derived with the subclasses `MoldingOperator`, and `SimulationRun`. A production asset is captured by `VDIProductionAsset` with subclasses such as `Workstation` and `SimulationTool`. A larger challenge is to capture the process flows and alteration of the input/output states. A complete process workflow is called `VDIProcess` and is a wrapper that includes the system limit, which has one or more `hasOperator` properties pointing to its initial `VDIProcessOperators`. The

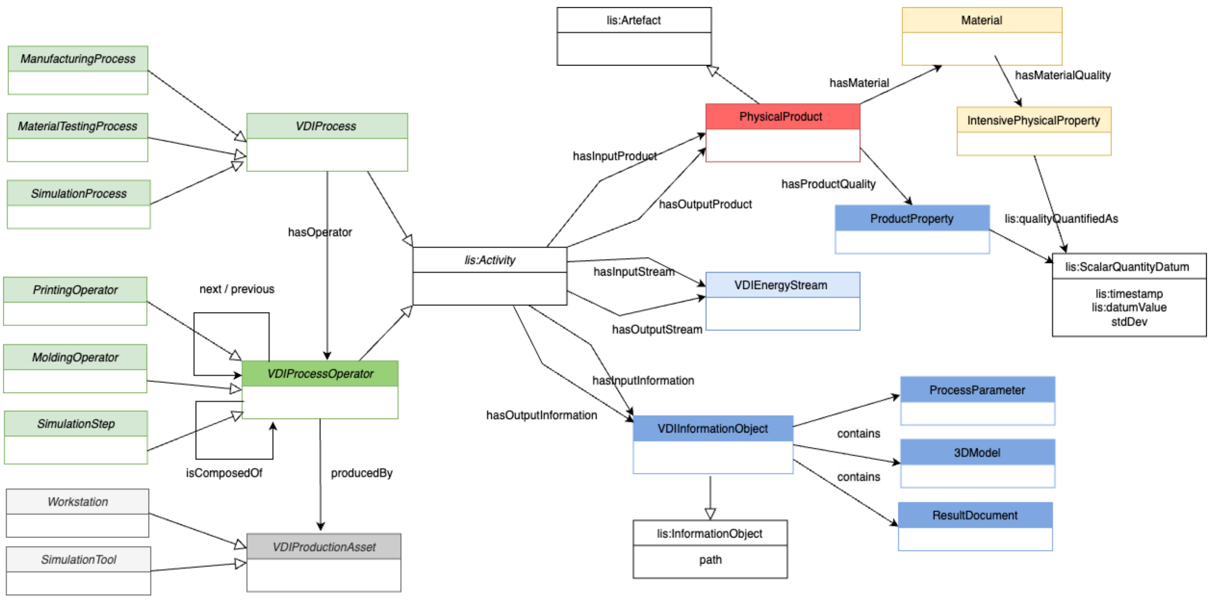


Figure 5: Partial rendering of VDI 3682 language elements in the ontology including the alignment with IDO and using the same color coding as in the standard.

properties `next` (and the inverse `previous`) define the next (and previous) evaluation order of a specific operator. The three states are linked to a `VDIProcessOperator` by the following object properties, whereas at least one state is required to be linked:

- product state: by `hasInputProduct` and `hasOutputProduct` to `PhysicalProduct` thus connecting products and their related materials to processes;
- information state: by `hasInputInformation` and `hasOutputInformation` linking to `VDIInformationObject`, which has a property `source` to underlying documents and can combine several process parameter or result items by the property `contains`;
- energy state: by `hasInputStream` and `hasOutputStream` to `VDIEnergyStream` class;
- technical resource: by `producedBy` with the domain `ProductionAsset`.

Our representation does not fully align with the VDI 3682 language, as some definitions seem redundant. We have not introduced any concept for the system border, since the `VDIProcess` represents the border. For example, any state connected directly to `VDIProcess`, e.g., by `hasInputProduct`, is the interface to the exterior of a process. Note that the VDI 3682 language does not have a next and previous relation to represent an explicit process flow. Hence, we introduced the `next` and `previous` object properties, since they should simplify the query of explicit process flows using property paths. The `next` property can be deduced by the property chain: $\mathtt{hasIP}^{-} \circ \mathtt{hasOP} \sqsubseteq \mathtt{next}$, where `hasIP`, `hasOP` and `next` represents `hasInputProduct(y,z)`, `hasOutputProduct(x,z)`, and `next(x,y)`.

4.4. Usage Example

To illustrate the use of the OMO, we give a simple example of a knowledge base (KB) that describes a test specimen used in the OntOMat project. A test sample is produced by resin transfer molding (RTM), where a liquid epoxy resin is injected under pressure into a closed mold containing dry glass fiber, which is then cured to form a composite part, i.e., the resulting product.

First, we describe the material and its composition, and add the material quality density and its value measured in a material characterization process:

```
:epoxy-M_LY556_GFKUD0_01   rdf:type ontomat:CompositeMaterial ;
    rdfs:label "Siemens Epoxy GFK UD" ;
    ontomat:manufacturedBy "Siemens Technology" ;
    ontomat:hasMatrixWith   :araldite_LY_556 ;
```

```
    ontomat:reinforcedWith :acrystal_L_4040_BB ;
    ontomat:hasMaterialQuality :epoxy-M_LY556_GFKUD0_01-density .

:epoxy-M_LY556_GFKUD0_01-final-part rdf:type ontomat:FinalProduct ;
    rdfs:label "Epoxy GFK UD final part" ;
    ontomat:hasMaterial :epoxy-M_LY556_GFKUD0_01 .

:araldite_LY_556 rdf:type ontomat:EpoxyResin ;
    rdfs:label "Araldite LY 556" ;
    ontomat:manufacturedBy "Huntsman Corporation" .

:epoxy-M_LY556_GFKUD0_01-density rdf:type ontomat:Density ;
    rdfs:label "Density" ;
    lis:qualityQuantifiedAs :epoxy-M_LY556_GFKUD0_01-density-val1 .
:epoxy-M_LY556_GFKUD0_01-density-val1 rdf:type ontomat:MeasuredQuantityDatum ;
    lis:datumValue "1.79" ;
    ontomat:standardDeviation "0.01"^^xsd:decimal ;
    lis:datumUOM unit:KiloGM-PER-M3 .
```

Second, we outline the RTM process and a single process operator according to the VDI 3682 standard. Note that the RTM process has nine operators, but we only show the first one for brevity:

```
:epoxy-M_LY556_GFKUD0-MaterialForming-Main rdf:type ontomat:ManufacturingProcess ;
    rdfs:label "Epoxy GFK UD Process" ;
    ontomat:hasOperator :epoxy-M_LY556_GFKUD0-MaterialForming-PO01, :epoxy-M_LY556_GFKUD0-
        MaterialForming-PO05 ;
    ontomat:hasInputProduct :araldite_LY_556-product-1, :acrystal_L_4040_BB-product-1 ;
    ontomat:hasOutputProduct :epoxy-M_LY556_GFKUD0_01-final-part .

:epoxy-M_LY556_GFKUD0-MaterialForming-PO01 rdf:type ontomat:VDIProcessOperator ;
    rdfs:label "Epoxy GFK UD process for compressing" ;
    ontomat:hasInputProduct :araldite_LY_556-product-1 ;
    ontomat:hasOutputProduct :araldite_LY_556-product-2 ;
    ontomat:producedBy :pressure_vessel-asset-01 ;
    ontomat:next :epoxy-M_LY556_GFKUD0-MaterialForming-PO05 .
```

Third, we modeled a generic simulation process according to the VDI 3682 standard. This process model can capture several types of simulations, such as structural mechanics simulations, using finite element analysis software. As illustrated in Figure 6, a generic simulation process can be described as a preprocessing, a simulation (that is, running the simulation), and a postprocessing operator. A material instance (e.g., a specific fiber-reinforced epoxy resin), a geometry (e.g., the shape based on a given standard) and a set of input parameters are the input states, while the simulation results (e.g., additional material qualities), information (e.g., logs), and a simulated specimen (of a material) are the output states of the simulation process. Note that we deliberately modeled a material instance as a (specified) physical object instead of an information object. Furthermore, this process model does not suffice to describe multi-scale simulation processes, which could be seen as a parent process with the above simulation process as one of several compositions.

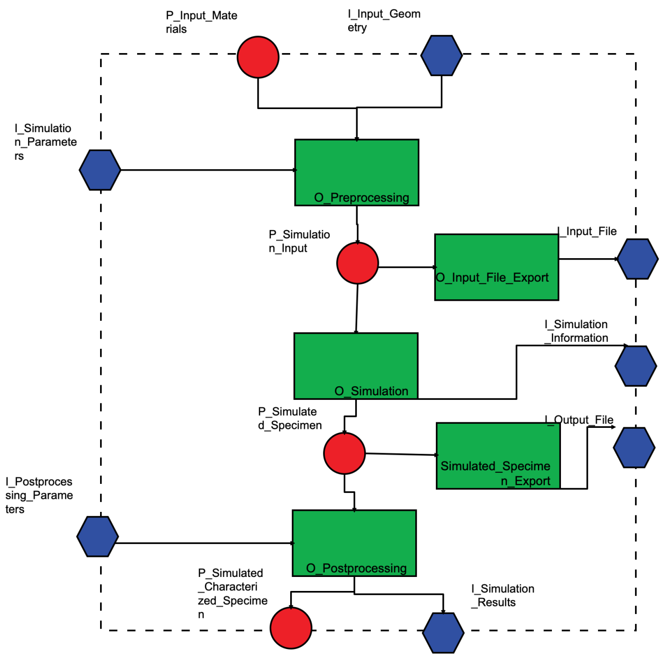


Figure 6: A generic model of a simulation process.

From this simple example, one can see that it is not feasible to create and maintain instances for more complex processes manually. Thus, the next step in the OntOMat project is to provide tools for data onboarding of VDI 3682 process models created with the FPB.JS tool[11] of Fay et al. [13]. Additional sources such as input parameter, source, and log files that describe the boundary conditions or process parameters of a specific simulation run can be used to enrich the imported models.

5. Discussion and Conclusion

In this paper, we outline the ontology development process in the OntOMat project and introduce the main elements of the resulting OntOMat ontology. Describing base material classes and material properties is as expected, but modeling and import of the IEC 62474:2018 standard, as well as the related equality axiom-based classification of composite materials, based on their base materials, is a novel approach to material classification. At the core of the OntOMat ontology is the representation of the VDI 3682 (Formal Process Language) standard, which is a visual language to describe any kind of real and digital processes. Due to the complexity of the VDI 3682 standard, it is not trivial to find an appropriate semantic representation of it. However, this should allow us to describe complex multiscale simulations, integrate the results of these simulations, and align them with underlying material systems.

We recognize that the current ontology has limitations and still needs to be extensively evaluated with real characterization, simulation, and manufacturing processes. One limitation is that we do not fully support parallel process flows, which require additional concepts such as synchronization points. The axioms for automatically deducing the object properties `next` / `previous` and the automatic classification that the processing states are in the limit of the system are yet missing. Furthermore, technical resources are coarse-grained modeled, and a taxonomy based on the ISA-95[12] standard would be valuable.

The future work focuses on several directions: (a) finalizing the ontology addressing the above limitations and a complementary alignment to the PMD Core Ontology; (b) providing an extensive tool set for injecting data for specific material systems based on input spreadsheets; (c) supporting the integration of existing VDI 3682 visual process modeling tools; (d) in addition to an existing SPARQL interface, also provide a GenAI-based copilot to interact with the knowledge base combining the ontology with instances for each material system.

Declaration on Generative AI

During the preparation of this work, the authors used Writefull for Overleaf[13] to check grammar, spell check, and paraphrase to improve the readability of the text. The authors reviewed and edited every suggested content improvement and assume full responsibility for the content of the publication.

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