Advanced Engineering Materials

ADVANCED ENGINEERING MATERIALS
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RESEARCH ARTICLE OPEN ACCESS

OntOMat: Toward Ontology-Based Product and Process Design Engineering and Optimization Solutions Fueling Circular Value Chains

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Received: 8 April 2026 | **Revised:** 22 June 2026 | **Accepted:** 23 June 2026

Keywords: digital twin | fiber reinforced plastics | formalized process description | material extrusion | multi-scale modeling | ontology/knowledge graph | product life cycle

ABSTRACT

This study presents concepts and modeling patterns for the materials and process domains of polymer matrix fiber reinforced composite materials in the context of industrial products. Manufacturing processes covered include injection, hot compression, autoclave molding, resin transfer molding (RTM), and material extrusion (MEX). Characterization processes, i.e., X-ray computed tomography (CT), digital holography, and mechanical testing, are modeled and applied for data generation. Physical and virtual product models are described, including multiscale design and process engineering, the latter illustrated using a MEX process. All processes are modeled using the VDI/VDE 3682 formalized process language to ensure interoperability and structure data aggregation. The material modeling concept separates intensive and extensive properties and reflects the hierarchical structure of composites, including distinct interphase modeling. The IEC 62474 classification is adopted and expanded to capture specifics of polymer matrix fiber reinforced composites. These concepts are implemented in the OntOMat ontology (OMO) using the web ontology language (OWL). Competency questions serve as requirements for ontology development and evaluation. Finally, the resulting knowledge graph is combined with a large language model to provide an interactive user interface and API based on SPARQL.

1 | Introduction

Innovative industrially manufactured products rely on the development of high-performance materials and their respective fabrication processes. However, a continuous and comprehensive digital model of the relationships between material/material properties, processes, and component/product is not available. Likewise, there is no data integrity and interoperability between the respective characterization, simulation, and manufacturing processes, which prevents the consistent use of the resulting data and its application to the development of artificial-intelligence (AI)-based digital assistants [1]. The development of a harmonized ontological description can remedy this situation and thus open up new potentials for data-driven material development, process optimization, and the implementation of circular product value chains using knowledge graphs.

The starting point for the work described within this study is a digital material description, as conceptualized in Figure 1.

Within the BMFTR (Federal Ministry of Research, Technology and Space) funded project OntOMat, the example of fiber-reinforced polymer matrix composite materials and their related processes was then adopted to develop a first version of such digital material description, aiming to model materials in the context of industrial products and their respective product life cycles. The goal being to obtain a digital material description, respectively, ontology/knowledge graph, that allows for the optimization of the product's design, fabrication, operation, and end-of-life performance, as well as the related workflows. Tying in with that, this paper is not addressing any new material or process development but rather tries to model the domain based on industrial standards, commercially available materials, and industrial grade manufacturing and characterization processes. Moreover, no specific product or product design is presented, the physical artifacts are limited to test specimen and samples. The aim is to make the results, especially the developed ontology directly applicable to industrial practice and to evaluate the performance of the ontological description and framework with respect to existing knowledge. Currently, the work presented is not focused on supply chain and procurement, substance compliance, product service life, shop floor management or energy efficiency aspects. Chapter 2 describes the physical materials and processes underlying the ontology and respective knowledge graph development, and Chapter 3 outlines the modeling domain and modeling patterns that provide the base for the developed ontology. Chapter 4 illustrates the implementation of the OntOMat ontology (OMO) and knowledge graph (KG) as well as data ingestion pipelines to create a KG and three prototypical user interfaces to interact with it.

Existing ontologies and knowledge graph initiatives in materials science provide important building blocks, but they do not yet offer a domain-refined representation of fiber-reinforced polymers (FRPs) that tightly integrates processing, structure, properties, and simulation. At the upper level, the Elementary Multiperspective Material Ontology (EMMO) [2, 3] and related efforts within the materials modeling community provide generic, physics-based patterns for representing materials, processes, and properties, but they are intentionally domain-agnostic and require substantial specialization to capture the heterogeneous, anisotropic nature of FRPs and their complex manufacturing routes. Earlier materials ontologies, such as the Materials Ontology by Ashino [4], demonstrated how formal semantics can support exchange and integration of materials data, but they primarily target crystalline and metallic systems and do not explicitly model composite-specific architectures or process-induced defects. In chemical and process engineering, OntoCAPE [5] illustrates how detailed process ontologies can be built and reused across applications, yet its focus lies on continuous process plants rather than discrete manufacturing steps such as fiber placement, resin infusion, or curing of polymer composites. Large-scale data infrastructures like the Novel Materials Discovery (NOMAD) Laboratory [6] and related efforts toward FAIR materials data management emphasize schema, metadata, and provenance for computational materials science and have inspired knowledge-graph-based approaches in materials informatics [7]. However, they typically concentrate on composition-structure-property relationships derived from electronic-structure or atomistic simulations, with only limited coverage of manufacturing process chains. A Unites States federal, cross-agency program launched in 2011, the Materials Genome Initiative (MGI) [8] promotes faster and more cost-effective discovery, development, and deployment of new materials by coordinating advanced modeling, computational tools, and experimental data within a shared framework. Within the German materials data ecosystem, Platform MaterialDigital [9, 10] has introduced core ontologies and data models for FAIR materials data and workflows, but current public documentation still offers only high-level concepts for composites and processing steps, without a dedicated, FRP-specific ontology that (i) captures constituents, architecture, and process history across scales; (ii) integrates experimental and simulation workflows in a unified representation; and (iii) supports explicit, machine-actionable process-structure-property relationships. Related projects within the Platform MaterialDigital include SensoTwin [11], which in contrast to OntOMat focuses directly on a single component, i.e., a wind turbine blade, while the scope of OntOMat is more generic. The ontology and knowledge graph presented in this work are designed to address precisely these gaps within the MaterialDigital framework, with a specific

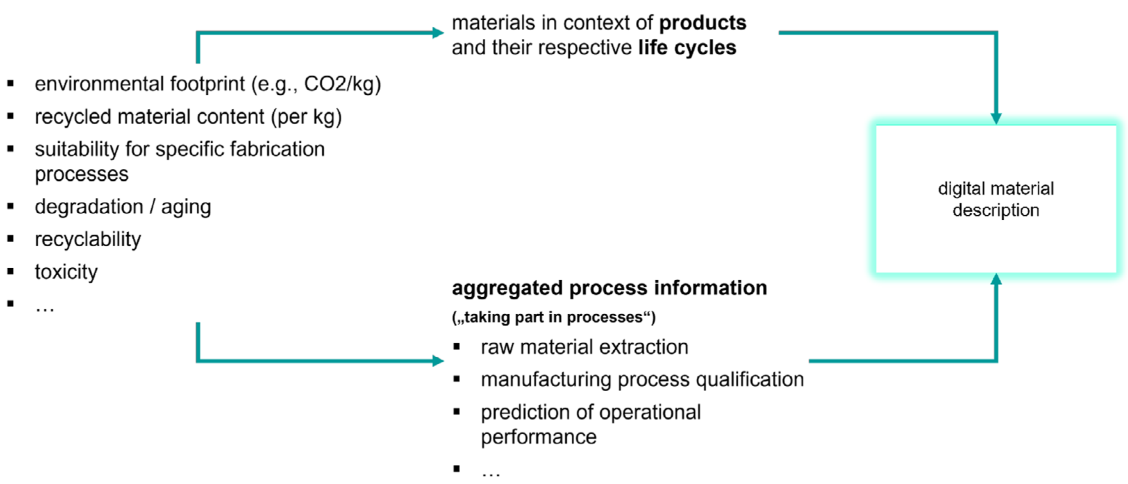


FIGURE 1 | Extension of digital material description beyond physical material properties.

focus on fiber-reinforced polymer systems and the prediction of effective properties.

2 | Context and Specification of Modeling Domain

Following the concept shown in Figure 1, a material "takes part" in several processes during the product life cycle, giving rise to material attributes that go far beyond the well-known physical material properties. Obviously, for those "process-related" properties, the property values can undergo continuous change with each process participation, like the CO_2/kg equivalent or the recyclability rate of the materials. However, this is equally true for the (classical) physical material property values, which are also dependent on the processes the materials are taking part in. Typical examples for processes that potentially change the physical property values of product materials are manufacturing processes and the degradation during the product operation phase. Hence, describing and modeling materials in context of products is expected to result in a harmonized and generic digital material model.

The material class/system of fiber-reinforced polymer matrix composite materials provides a concrete and rich specification of the digital material modeling domain (see Chapter 2 for details of the modeling pattern). This can be attributed to the complex structure of the material system and the observed strong dependency of the material property values on the fabrication processes, resulting in the development of versatile design engineering workflows, including multiscale simulation, as well as in and ex situ characterization methods. To reduce complexity and improve the systematic description of material and process properties, a multiscale modeling approach is adopted for the domain ontology development. This enables the modeling of material properties in a substance-homogeneous manner and a direct transfer from the micro- to meso- and finally macroscale. The chosen material system as well as the considered processes are described in detail below.

2.1 | Physical Material Systems

Fiber-reinforced polymers (FRPs) are a class of composite materials consisting of continuous or discontinuous fibers embedded in a polymer matrix. Within this material concept, the fibers form the main stress-carrying constituent, providing both stiffness and strength to the composite material, whereas the matrix supports and supplies cohesion to the fibers and protects the fibers from environmental impacts. When stiff glass [12] or carbon [13] fibers are used, FRPs achieve very high specific stiffness and strength, allowing substantial weight savings. Consequently, FRP materials are widespread in lightweight structural applications [14].

The macroscopic properties of FRP materials and other composites strongly depend on their microstructure. Due to the inherent microscale heterogeneity of the material, its effective properties are strongly influenced by the manufacturing process [15]. Different processing routes result in different fiber orientation states and fiber length distributions, which directly affect the effective thermomechanical response [16]. Consequently, establishing robust relationships between material properties and the full material and product history, including the manufacturing and processing cycles, is of central importance.

Traditionally, the matrix material has been a thermosetting polymer, which severely hampers recyclability. The use of thermoplastic matrices improves the feasibility of recycling and, therefore, is the focus of extensive contemporary research [17, 18]. However, recycled composites typically exhibit altered properties compared to virgin materials [19], further underscoring the need to track the complete product life cycle, material sources, and processing history when assessing and predicting the effective properties of FRP materials.

In the present contribution, different thermosetting and thermoplastic material systems are investigated. Thermoplastic materials can be re-melted repeatedly and are therefore very suitable for processing in the material extrusion (MEX) and the injection molding process (for details, see Section 2.2). The material properties heavily depend on the processing conditions, especially the cooling rate. The three thermoplastic material classes investigated are specifically tailored to be used in a granule based material extrusion process:

- A partly recycled glycol-modified polyethylene terephthalate with a short carbon fiber content of 15% (rPETG CF15) represents the class of standard to low technical grade thermoplastics. Typical processing temperatures for this amorphous material are around 230 °C. Additionally, the composite material will be used fully recycled after a further recycling step.
- As a representative of a technical thermoplastic material, a semi-crystalline polyamide 6.6/6 blend is investigated. It is a 25% glass fiber-reinforced material and provides flame-retardant properties (PA66/6 GF25FR) according to DIN EN 45545-2 R1 HL2 which is suitable for a wide range of applications in rail vehicles. Its processing temperature is approximately 280 °C.
- The group of high-performance thermoplastics is covered by an amorphous polyetherimide. It has a short carbon fiber fraction of 20% (PEI CF20), is usually used to produce high-temperature toolings and molds and processed at around 350 °C.

Epoxy fiber prepregs are a thermosetting material system consisting of epoxy resin impregnated unidirectional, woven or chopped carbon or glass fiber fabrics. Once cured, the epoxy matrix cannot be remelted. Although there are fast-curing material systems that cure within 3 min, standard epoxy resins generally only reach their gel time (time to take on the intended shape) after a period of 30 min to several hours, depending on the temperature used. Hence, in contrast to thermoplastic material systems, they are not suitable for material extrusion processes and are typically processed in compression or autoclave molding processes (for details see Section 2.2). This material system is often referred to as sheet molding compounds (SMCs). The following material classes have been investigated during the project:

- HexPly M21 is a toughened fiber filled epoxy resin system. It has a high performance, very tough epoxy matrix for use in primary aerospace structures. It is typically processed at 180 °C. In the material description within the project, the toughener is understood as an additional filler for the epoxy matrix. As part of the investigations, the following specific materials were selected, which have a relevant technical application in technical applications and, above all, represent different aspect ratios on the length side of fiber reinforcements:

- Hexply 8552: Prepreg material system consisting of thermosetting epoxy resin matrix and continuous carbon fibers; processing takes place in pressing and autoclave processes
- Araldite LY556/HY906 + glass/carbon fibers: Thermosetting CFRP systems are based on epoxy resin and continuous glass/carbon fibers; processing is carried out via resin injection process (infusion or resin transfer molding).
- VERKID ASTAR VG03-60 GF: Sheet molding compound (SMC) consisting of a vinyl ester matrix and long glass fiber reinforcement; processing is carried out via hot compression molding, rarely in an autoclave process.
- Celstran GF50: Injection molding material system consisting of a thermoplastic polypropylene matrix and long glass fibers (50 wt).

2.2 | Physical Processes

2.2.1 | Physical Manufacturing

Material extrusion is an additive manufacturing process defined in DIN EN ISO/ASTM 52900 [20]. Process preparation typically involves a slicing step, during which machine instructions are generated from a given three-dimensional model. These instructions are based on predefined process parameters such as strand geometry or deposition strategy and consist of a number of target positions and tool orientations along with target extrusion rates, travel speeds, and further (custom) information if necessary (so-called G-Code, see [21]). For processing, thermoplastic material—commonly supplied in pellet form—is first dried and subsequently conveyed into a single-screw extruder. Within the extruder, the combined action of shear forces and thermal energy plastifies the material, enabling extrusion through a nozzle. A kinematic system, such as a robotic arm or gantry system, continuously positions the extruder to deposit the molten polymer with controlled strand geometry, usually in a layer-wise manner. Progressive solidification of the deposited material leads to the formation of the final component. The robotic facility used for the MEX process is depicted in Figure 2. Depending on the material, component geometry, and deposition path, the introduced thermal energy is a critical factor for achieving the intended geometry and the desired material properties, particularly for semicrystalline thermoplastics. In addition to pellet-based systems, the MEX process can also be filament-driven, which enables not only short-fiber reinforcement but also the manufacturing of components with continuous fiber reinforcement.

Hot compression molding is a process where preheated polymer or composite material is placed into an open, heated mold. The mold is then closed and compressed with high pressure. Heat and pressure force the material to flow and fill the cavity, curing or solidifying it. Once the cycle finishes, the mold opens, and the final part is removed. With this technology, the material system SMC and partially prepreg are processed.

Autoclave molding is a high-precision composite manufacturing method commonly used with prepregs. Layers of fiber prepreg

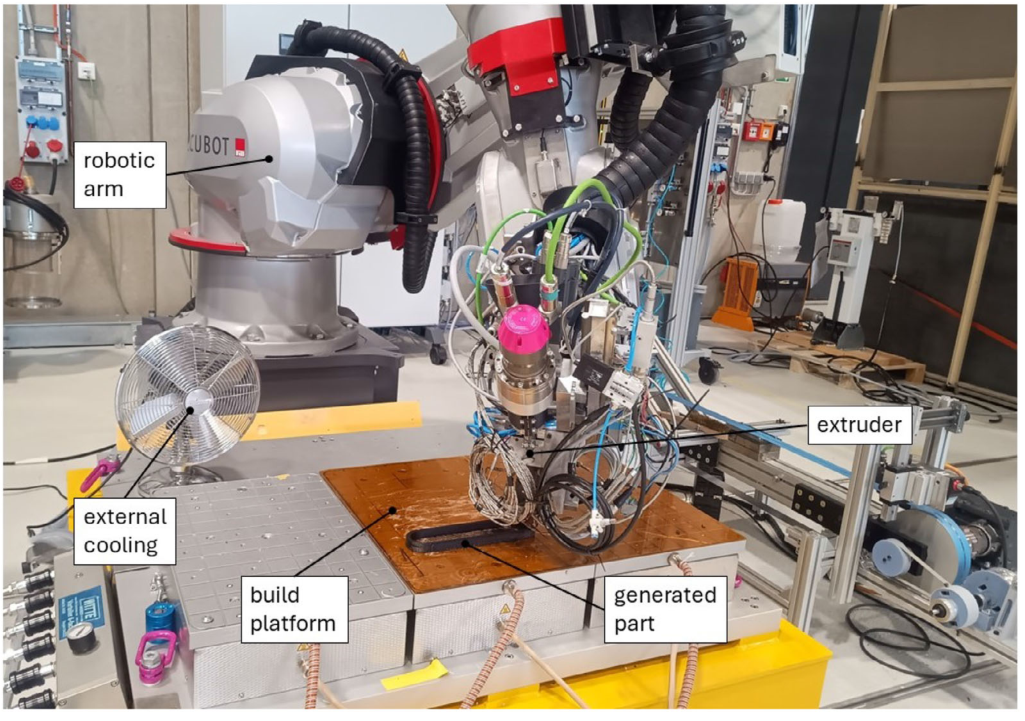


FIGURE 2 | Mid-operation of a MEX process. A robotic arm continuously positions a single-screw extruder, which deposits molten thermoplastic polymer and thus, generates a part.

are placed on a tool and sealed with vacuum bagging. The assembly is placed in an autoclave, where vacuum, heat, and high external pressure consolidate and cure the laminate. With this technology, the material system prepreg is processed [22].

Resin transfer molding (RTM) is a closed-mold composite process using dry fiber preforms. A dry preform is positioned inside a closed mold. The mold is moved into an RTM press (as shown in Figure 3) to be heated, where liquid resin is injected under pressure, impregnating the fibers. The resin cures in the mold, after which the part is removed. With this technology, the material Araldite is processed [23].

FIGURE 3 | RTM press as part of the automated “EVo” production line at DLR Stade, equipped with a mold-transfer-system connecting demolding station, press and oven. In this case, it will also be utilized for compression molding to process SMC material.

Injection molding is widely used for thermoplastic parts. Plastic pellets are melted in a heated barrel. The molten material is injected under high pressure into a cooled mold. The material solidifies, and the part is ejected. With this technology, the material PP Celstran is processed [23].

2.2.2 | *Characterization*

Advanced X-ray-based nondestructive testing methods, as shown in Figure 4, were used for offline (ex-situ) microstructural characterization of fiber-reinforced test specimen manufactured by compression and autoclave molding processes, as well as material extrusion (MEX) and injection molding processes. X-ray CT (CT) was performed to obtain 3D volumetric images of the entire test specimen for the detection and quantification of microstructural features such as pores, cracks, and delamination. Conventional computer tomography allows the segmentation of glass-fibers and their separation from the surrounding matrix. However, carbon fibers and the surrounding matrix have similar densities. Therefore, the segmentation of carbon fibers with conventional CT is challenging. On the other hand, X-ray microscopy (XRM) was performed for high-resolution region-of-interest (ROI) measurements [24] and propagation-based phase contrast. The corresponding setup is shown in Figure 4b. XRM allows the segmentation of carbon fibers and their separation from the surrounding matrix. This workflow was performed in volume graphics, enabling detailed analysis of microstructural features such as fiber orientation, fiber length, and early damage initiation.

Talbot-Lau grating interferometry (TLGI) (see Figure 4a) was employed to complement conventional CT by increasing sensitivity to low density differences and subresolution features, and it was used in particular to detect microcracks and fiber-related damage. Three complementary contrast modes were acquired with TLGI: absorption contrast (AC), differential phase contrast (DPC), and dark-field contrast (DFC) [25]. The image data was segmented and processed into quantitative descriptors,

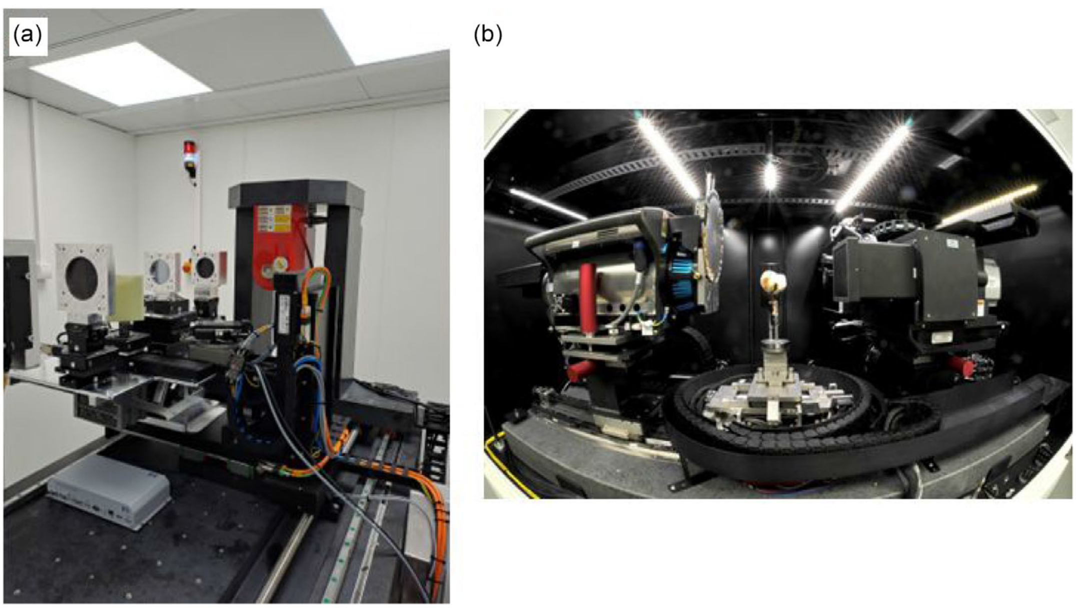


FIGURE 4 | (a) X-ray cabin with experimental platform (funding code 49IZ240042) for TLGI (funding code 49IZ190032) and conventional CT and (b) X-ray Microscope (MAPEX, University of Bremen): X-ray source (left), cotton seed (specimen middle) and detector (right).

including pore volume fraction, pore size and spatial distribution, fiber volume content, and fiber-orientation tensors.

Failure and damage evolution under cyclic mechanical loading were investigated by combining in-situ CT with digital volume correlation (DVC) to quantify internal strain fields and damage progression. These results were coupled with acoustic emission measurements and numerical failure simulations to enable virtual testing and validation of simulated failure behavior. All image processing and quantitative analyses were performed using Volume Graphics (VGStudio MAX 2025/4). The resulting datasets provided global quality metrics for production process validation (e.g., pore volume fraction) as well as high-resolution reference data for multiscale material, process, and failure simulations.

Digital holography [26] is used to provide in-line (in situ) imaging and profile characterization during filament based additive manufacturing processes. It is an interferometric imaging method, which is based on recording interference patterns directly on a camera sensor, i.e., the digital hologram, between light scattered by the specimen and a reference wave. From the hologram, the image of the object can be numerically calculated. The great advantage of digital holography is that it does not require lenses for the imaging process, which enables unusual imaging geometries, e.g., to observe the sample from an oblique angle, or to digitally select the imaging area. In the framework of our investigations we developed a new imaging method, "Sideways Lensless Imaging" (SLIM) [27]. It offers unusual and flexible adaptations of the imaging geometry, which is especially convenient for in-situ measurements. Moreover, the method also provides a very high light efficiency, that is required in the context of PETG-parts from industry-scale 3D-printing, as the 3D-printed parts often feature a high surface roughness and in our case also very high absorption. The corresponding experimental setup of the *sideways lensless holographic interferometer* is shown in Figure 5a. The remarkable feature is the oblique observation angle of $\alpha = 29°$ due to the laterally shifted sensor position. Figure 5b shows a resulting reconstruction of the recorded 3D-printed PETG-part. The measurement data from this optical characterization method will be used for in situ shape measurements to characterize the physical object.

Conventional mechanical characterization of test specimen manufactured by the processes described in Section 2.2.1 are performed via tensile tests according to standard DIN EN ISO 527-4 and inter laminar shear strength (ILSS) tests according to DIN EN ISO 14130. These static characterization methods allow the determination of the elastic moduli in different directions as well as tensile and shear strength properties, which are commonly used to characterize fiber reinforced composites. All material tests are performed on Zwick/Roell machines using the TestXpert Software on test specimen in dog bone shape of type 1B. An API allows the Software to write all test results directly to a Shepard-Database[1] for further analysis. As the process induced fiber orientation is in general not isotropic, anisotropic material properties are expected. Hence, the test specimens are tested in two different orientations, the 0° and 90° directions relative to the preferred fiber alignment. The determination of interlaminar shear strength primarily provides information about the layer adhesion of the composite. The shear stresses that occur can cause a break between the fiber and the matrix. Test specimen are therefore characterized in a 3-point bending setup with very short support distances. Here, the orientation of the fiber reinforcement is also crucial.

2.2.3 | *Multiscale and Processing Simulation Workflows*

In modern product development, it is common to use virtual methods (Computer-Aided Engineering) to support the product creation process. The finite element method (FEM) plays an important role in this context, as it enables components and materials to be designed virtually and tested under various loads. By using FEM simulations, the development process can be accelerated, physical tests can be reduced, and costs can be saved

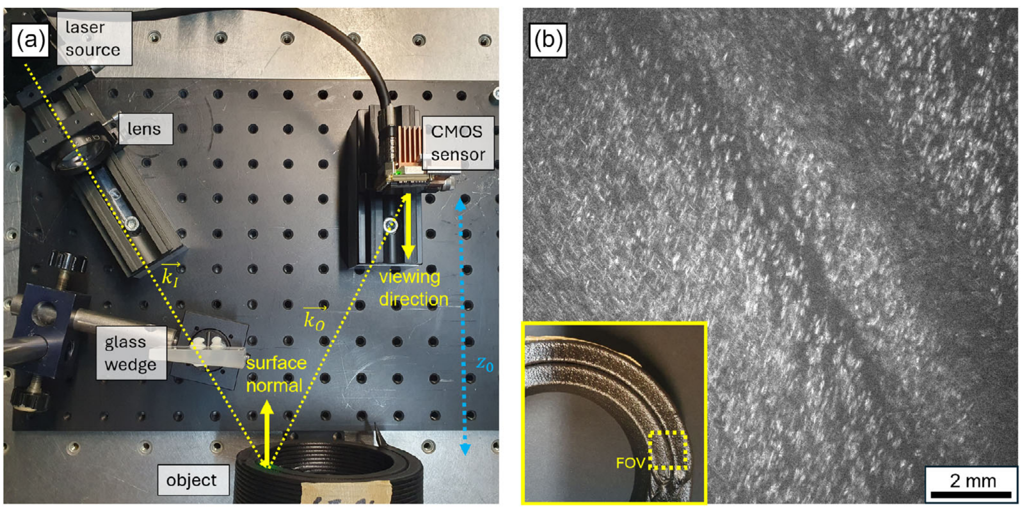


FIGURE 5 | (a) The *sideways lensless holographic interferometer* used for the measurement of a 3D-printed PETG-part. It features a triangular geometry chosen symmetrical in respect to the surface normal of the object, with the illumination direction $\vec{k}_I$ and the observation direction $\vec{k}_O$. Noticeable is the laterally shifted sensor position at a distance of $z_0 = 170$ mm from the object plane, giving an observation angle of $\alpha = 29°$. The glass wedge is used to provide reference wave and object illumination by splitting the illumination beam. (b) Resulting holographic reconstruction of the recorded 3D-printed part. The corresponding field-of-view (FOV) is shown in the insert [27].

[28]. Current developments aim at creating a digital twin of a product or even a material, which can be used to plan manufacturing processes and monitor subsequent operation. A major challenge in the numerical design of composite materials is their heterogeneous, direction dependent mechanical behavior and the pronounced differences in the properties of their constituents [29]. To provide a basis for the calculation of composite components, various homogenization methods have been developed that build on the fiber volume fraction. Examples include the methods of Chamis or Puck [30]. For a more detailed investigation of the mechanical properties of fiber reinforced polymers, a numerical FEM simulation can be used. Compared to classical mixture rules, this method offers the advantage of being able to incorporate micromechanical processes and characteristics such as fiber arrangements, fiber matrix interfaces, pores, as well as crack initiation and propagation mechanisms [31]. As current computing capacity is not sufficient to run a FEM simulation of all fibers within a part, the usage of a multiscale approach is used in simulation. Here, at first, a microscale representative volume element (RVE) is created in a way that the whole part can be built by assembling this RVE. This means that the arrangement of fibers and pores in this RVE should correspond as closely as possible to their arrangement in the actual component. Now, the FEM simulation is carried out using this RVE at the microscale. The homogenized mechanical parameters obtained from this analysis are then transferred to a RVE on the next higher scale level which often contains a cut-out of the fiber fabric. The homogenized properties from this mesoscale analysis are then transferred to the part model which then can be simulated without the need to model every single fiber [32]. A schematic representation of the multiscale simulation is shown in Figure 6.

Besides the material and part focused simulation work flows, a processing simulation is carried out for the MEX process. The achievable material property values of MEX printed parts are strongly influenced by the temperatures during solidification of the beads, which are governed by the process parameter specification. For example, warping behavior or interlayer adhesion strongly depend on the process parameter specification for printing speed or bed temperature. Hence, simulations of the temperature distribution in dependence of the deposition process parameters allow for the analysis of the achievable part quality and to maximize process performance. To achieve this, the respective FEM simulation uses the real G-code of the printing process and activates elements at the same coordinates and at the same time as in the real printing process, resulting in a virtual 3D print of the part. During this layer-by-layer process, the material orientations are continuously updated based on the deposition direction, while dynamically changing surface conditions. The surfaces exposed to air cooling and those embedded within the material are updated analogously to the material orientations. An example of such simulation of a MEX process is shown in Figure 7.

Summarized, the virtual print can be used to calculate the temperatures and eigen-tensions to reduce physical printing trials and scrap parts.

2.2.4 | *Product Material Circularity*

Regarding product circularity, especially material recovery, two established recycling routes were investigated, and test specimens were fabricated using the respective material streams (for details, see Section 2.3). Hereby, one recycling route focuses on product end of life recycling, the other on recycling of production scrap.

In collaboration with the Sächsisches Textilforschungsinstitut e.V. (STFI), glass fibers from end of life wind turbine blades were identified as material stream (feedstock) for composite products manufactured by the RTM process (see sec. Section 2.2.1). Before the fibers can be provided to the RTM process, STFI processes them into nonwoven fabrics [33].

In collaboration with Kunststofftechnik Paderborn (KTP), production scrap resulting from material extrusion or injection molding processes was identified as material stream (feedstock) for composite products manufactured by injection molding and material extrusion processes (see Section 2.2.1). To prepare the production scrap for processing, KTP grinds it down to a particle size of 3–mm [34], making it directly applicable to conventional pellet conveying systems.

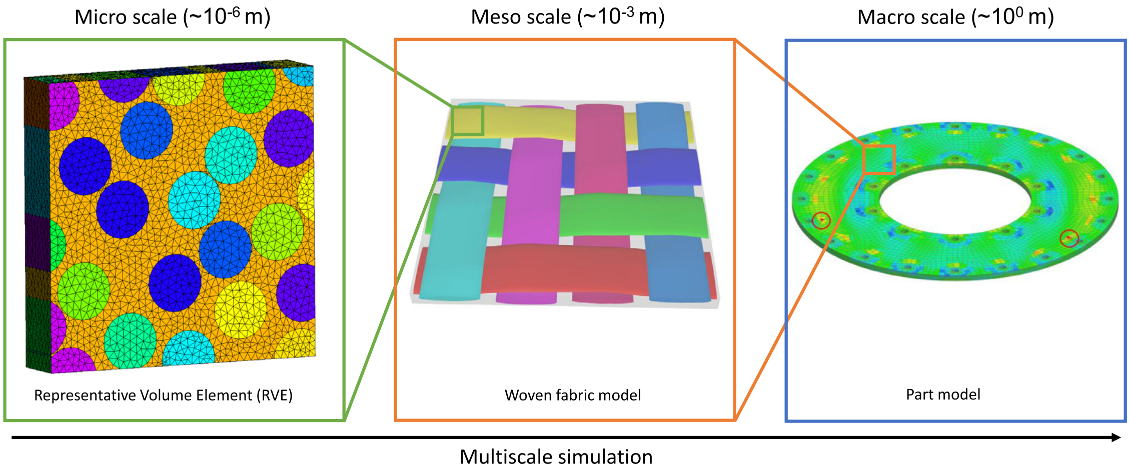


FIGURE 6 | Multiscale simulation scheme.

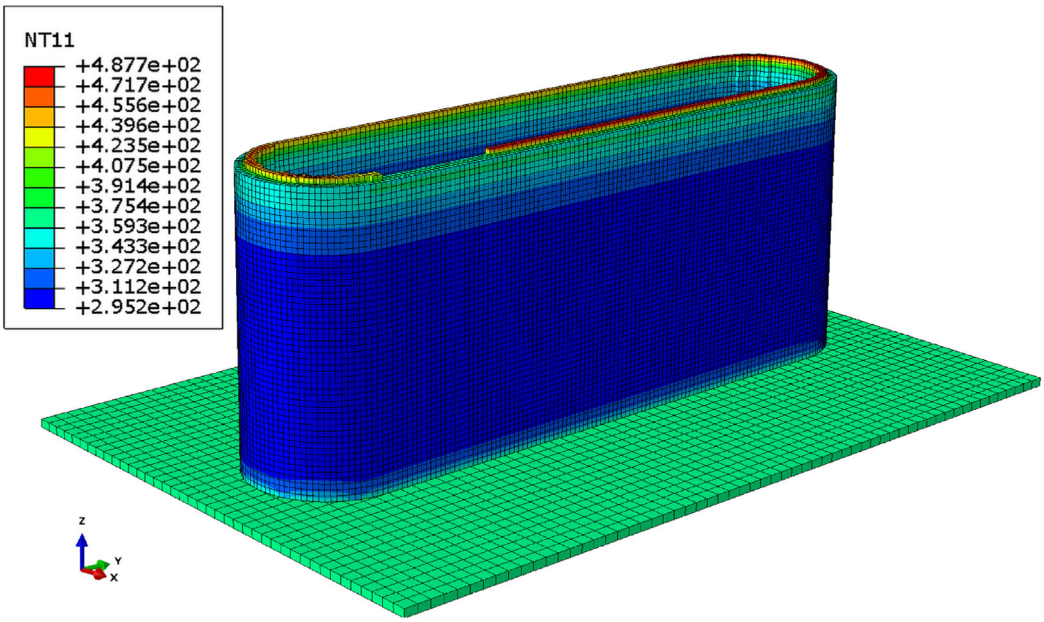


FIGURE 7 | Simulation of the temperature [K] distribution of a test part during the 3D printing process.

2.3 | Test Specimen Fabrication, Applied Characterization, and Simulation Workflows

To achieve a comprehensive data coverage of the domain of industrial grade fiber reinforced polymer matrix composites, including the various material systems, the fabrication and relevant in-situ and ex-situ characterization processes, as well as the applicable simulation workflows, a range of test specimen was fabricated, characterized, and subjected to simulation workflows (see Table 1). Details with regards to test specimen fabrication

TABLE 1 | Overview of fabricated test specimen, applied characterization and simulation processes.

Material system	Test specimen type/shape	Fabrication process	Characterization process	Simulation workflow
rPETG CF15	Stadium shape, dog bone	Material extrusion	X-ray, holography, tensile test	Processing
rPETG CF15 (regrind)	Stadium shape; dog bone	Material extrusion	X-ray, holography, tensile test	Processing
rPETG CF15	Plate, dog bone	Injection molding	Tensile test	n.a.
rPETG CF15 (regrind)	Plate; dog bone	Injection molding	Tensile test	n.a.
HexPly M21	Plate, dog bone	Compression molding	Tensile test	n.a.
PA66/6 GF25 FR	Stadium shape, dog bone	Material extrusion	X-ray, holography, tensile test	n.a.
PEI CF20	Stadium shape, dog bone	Material extrusion	X-ray, holography, tensile test	n.a.
HexPly 8552	Plate, dog bone	Autoclave molding	X-ray, tensile test	Multiscale
Araldite LY556 Aradur 906 DY070 CF	Plate, dog bone	Resin transfer molding	X-ray, tensile test	Multiscale
Araldite LY556 Aradur 906 DY070 GF	Plate, dog bone	Resin transfer molding	X-ray, tensile test	Multiscale
Araldite LY556 Aradur 906 DY070 GF (recylced)	Plate, dog bone	Resin transfer molding	X-ray, tensile test	Multiscale
VERKID ASTAR VG03−60 GF	Plate, dog bone	Compression molding	X-ray, tensile test	Multiscale
Celstran GF50	Dog bone	Injection molding	X-ray, tensile test	Multiscale
Celstran GF50 (regrind)	Dog bone	Injection molding	X-ray, tensile test	Multiscale

and process data acquisition are provided below, details regarding the specimen preparation for ex-situ X-ray characterization and tensile testing can be found in Section 2.2.2.

All test specimen fabricated by the MEX process are produced in the same manner. This applies to four different feedstocks: virgin rPETG CF15 pellets, rPETG CF15 regrind (see Section 2.2.4), virgin PA66/6 GF25FR as well as virgin PEI CF20 material. In the MEX process, these materials are processed using a 2 mm nozzle, generating the outline of a stadium shape structure. Three perimeters, adding up to a wall thickness of 6 mm, at a layer height of 0.8 mm are used to produce a part of 200 mm in height. Thus, for each material two straight walls of 200 mm × 200 mm form, which are subsequently cut out of the structure and face milled on either side to a final thickness of 4 mm. Tensile test specimens according to DIN EN ISO 527-4 Type 1B are then cut out of these. The orientation of the single specimens allows to assess the tensile properties in printing direction (see Figure 7, *y*-direction) as well as in vertical direction (see Figure 7, *z*-direction). The deposition process is recorded with a thermography camera for the rPETG CF15 and rPETG CF15 (regrind) stadium shaped specimen to measure the temperatures of the deposited polymer through the printing process. The resulting data is then used to calibrate and validate the process simulation described in Section 2.2.3. Moreover, all relevant machine parameters are recorded to enable subsequent correlation between the physical properties of the specimen and the manufacturing process. The monitored parameters include:

- Extruder and nozzle temperatures.
- Nozzle pressure.
- Nozzle position and deposition speed.
- Extruder screw rotational speed (RPM) and extruder torque.

For test specimen produced by injection molding, compression molding, and resin transfer molding, the process pressures, temperatures, and cycle times were recorded transiently. The property values of the test specimen were determined according to the applicable standards, specifically the mechanical properties in tension (ISO 527), bending (ISO 14125, ISO 178), and interlaminate (interlaminate laminar strength, ILSS (ASTM D2344)). Data acquisition for test specimen produced by compression molding was limited to pressure and temperature time series data during prepreg curing.

With resin transfer molding and autoclave processing, the project covers two of the most important manufacturing methods for structural components. The materials used were Araldite LY556 for the RTM process and Hexply 8552 for the autoclave process. As the basis for the subsequent characterization attempts, fiber-reinforced composite plates were manufactured using the Resin Transfer Molding process and the autoclave process. These plates are structured in such a way that they consist of several unidirectional layers. In the next step, specimens were milled from the plates in such a way that specimens with fibers oriented in the loading direction (0°), orthogonal to the loading direction (90°), and at a 45° angle were produced. The dimensions of the specimens comply with the ISO 527 standard. The use of plates with unidirectional fibers has the advantage that mechanical testing methods, such as tensile tests, can be used to specifically investigate the mechanical behavior of the composite in the fiber direction, transverse to the fiber direction, and at a 45° angle to the fiber direction. In addition, these specimens with known fiber orientations can be used to verify the accuracy of micro-CT analyses for determining fiber orientation. For parts with high production rates and moderate strength requirements, Sheet Molding Compounds (SMC) are a good choice. In their preprocessed state they consist of a paste that contains chopped fibers. A common manufacturing method to produce a part from that semi-finished product is compression molding. Here, VERKID ASTAR VG03-60 GF was used, and plates were manufactured from it using the compression molding process. Another important manufacturing process for composite components is the injection molding process. For this process, the GRP-material Celstran GF50 was used. In contrast to the RTM process and the autoclave process, no plates were manufactured here; instead, the test specimens were directly injection-molded using a suitable mold. In addition to the physical tests, a simulative characterization of the manufactured specimens was carried out using a multiscale FEM structural simulation. To validate the suitability of the simulation for determining the mechanical properties, exemplary simulation studies were carried out for unidirectional Araldite and Hexply specimens and compared with physical tensile and compression tests. The description of the multiscale simulation workflow can be found in Section 2.2.3.

Concerning the test specimen fabricated by material extrusion, digital holography was applied as in situ characterization, as described in Section 2.2.2. The corresponding workflow for planning and implementation of the characterization process is shown in Section 3.2.4.

3 | Domain Data Models, Modeling Patterns, and Process Descriptions

To achieve the goal of a digital material description that allows for the optimization of the product's design, production, operation, and end-of-life performance and the automation of the related workflows, a common domain data model relating the individual subdomains described in Chapter 2 is required.

3.1 | Domain Data Model

The domain data model provides the base for the ontology development and implementation (see chap. 4) and has been developed in a top down approach. As the starting point the underlying purpose of a product, namely the application, was defined. As an application directly implies the operation or use of a product providing a specific functionality for a certain time in a defined context or environment, this starting point was assumed to cover the entire product life cycle, as well as the aspects of product performance.

3.1.1 | Product Model

Figure 8 illustrates the developed physical and virtual product data models. As man-made industrial products are created to fulfill a specific purpose within a defined application, we

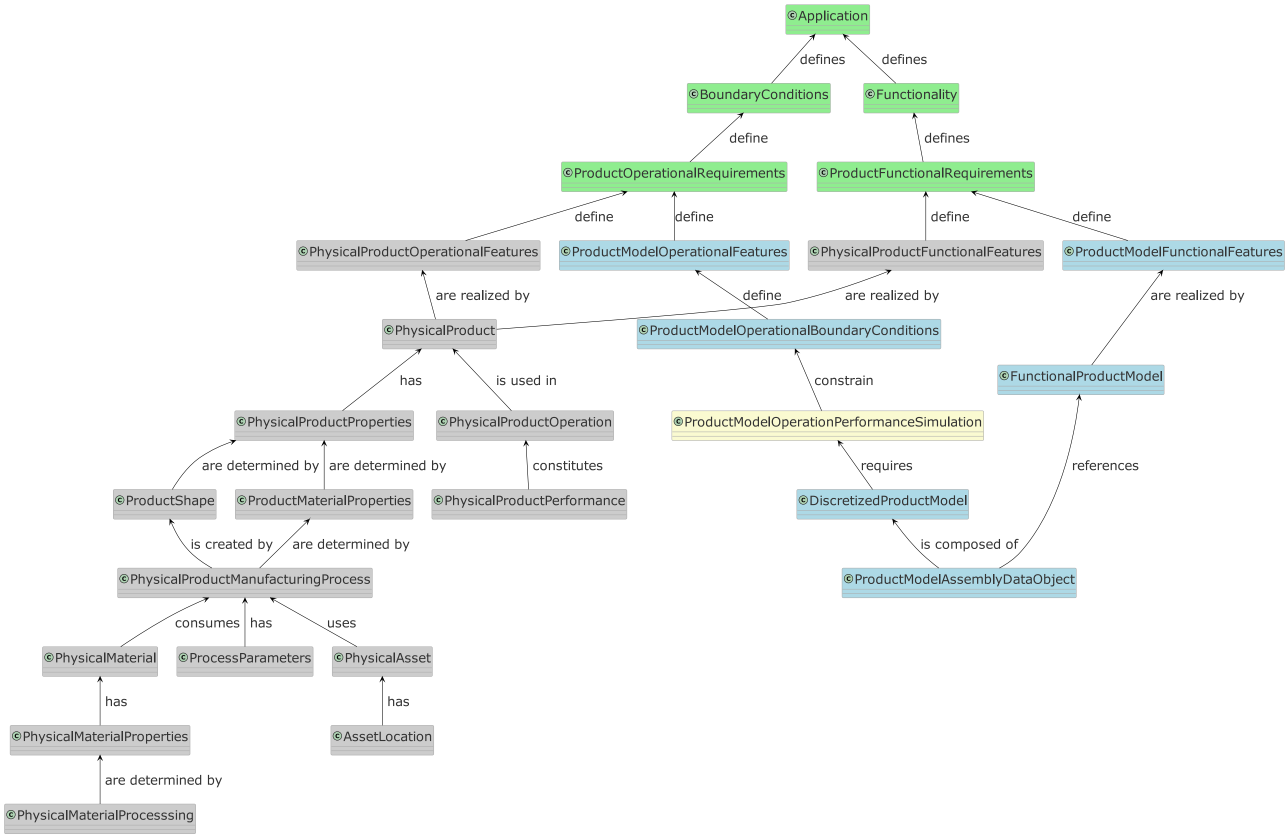


FIGURE 8 | Data model of physical and virtual products. Green color indicates requirement, gray color indicates physical product, blue color indicates virtual product (product model), and yellow color indicates performance related classes.

understand the product as the implementation of application requirements. Furthermore, we separate the requirements resulting from the specific application into functional and operational requirements. This is motivated by the fact that the function of a certain product needs to be provided by the product under certain boundary conditions, e.g., serving a drink on earth or in space. The functional and operational product requirements give rise to functional and operational product features, which are embodied by different product versions to different extents, resulting in the individual product properties of the physical products. We further separate these properties into product shape properties and product material properties, as this reflects the nature of physical material properties, specifically the separation into intensive and extensive properties (see Section 3.2.6). The product material and shape property values are the result of the product fabrication processes. It should be mentioned that, in certain instances, these processes can clearly be separated into shape changing and material composition/structure changing processes, but in general both properties are affected simultaneously. Input to the product fabrication process is the physical material, itself resulting from a material manufacturing process of either semifinished materials or raw materials (created by nonhuman processing). The operational product features embodied by the physical product constitute a product specific operation process or use (in dependence of the defined conditions). Besides the functional performance of the product, defined by the product properties, this provides the means to define the specific product operational performance as well as the product operational performance variation (e.g., the degradation), once measures and criteria are specified (see Section 3.1.4 for details). Clearly, during the product design phase, both aspects, the functional as well as the operational product features and the resulting performance need to be considered simultaneously.

3.1.2 | *Virtual Product Model and Design Engineering Chain (CAx Chain)*

As the virtual product model (commonly referred to as 3D product model or simply 3D model) is used to engineer and predict the product properties and performance of a to be fabricated physical product, it is designed to the same requirements as the physical product (see Figure 8) and will represent the respective features in terms of the specification of product model attributes and operational performance. Within the current industrial practice, the functional/manufacturing related aspects are often separated from the product operational performance aspects, resulting in two differently structured 3D product models, the functional and the discretized model, each representing individual aspects of the identical physical product. Both 3D models are the central part of the design engineering process and a joint optimization can be achieved via multidisciplinary optimization or agentic frameworks [35]. Common to both models is the creation of product geometry as a representation of the product dimensions. Using this geometric product representation, the functional and discretized models are created by enhancing it with additional information, e.g., product manufacturing information (PMI), connection information, or the surrounding or enclosed media. To predict the product performance with regards to its behavior in specific processes, e.g., via finite element simulation, the discretized product model is required. The functional product model represents the static functionality of a product, like shape (dimensions, surfaces, volumes), color, material, and PMI.

Using Siemens' NX software[2] as example, the structure of the data objects within the software application was examined and modeled (see Figure 9). This enabled us define the link between the materials and their properties to the different aspects of the product models as well as to provide the base for the calculation of statistical influences on the assessment of the simulation-driven product performance (see Section 3.2.5).

Regarding the interface to physical materials, the characterization of their properties as well as multiscale simulation hierarchy and part manufacturability, the here called material data object plays a significant role. Analogously to the geometric specification (i.e., dimensions) of the geometry body, the material data object holds one defined set of information about the properties of the material a specific volume body is made of. It contains analytical material models and their respective parameters as well as intensive physical material properties that can be specified by the respective material property values for a specific material. The material data object can exist at all scales. On macro- or part-scale, it references the continuum material properties and material models; on meso- or microscale, it references the individual properties of the constituent materials (e.g., the polymer matrix and the fiber reinforcement). As the material property and parameter values are usually derived by the characterization of physical material test specimen (material test data), the respective materials need to physically exist already. Hence, the material object, if populated with experimental derived material data, can be considered a limitation of the virtual product model's planning or prediction capabilities as it is tying it back to physically existing materials. As an alternative, the material data object can be populated by virtually derived material property values based on a discretized model of the material at meso- or microscale. In case of composite materials, a so-called representative volume element (RVE), that, e.g., represents the composite material constituents and their interface, is used to determine the mirco structural material performance under certain conditions (see Section 2.2.3). The obtained anisotropic material property values can be homogenized to represent continuum material property values, which can then be treated equally to the experimentally derived values. This can even include virtual testing of virtual test specimen to populate the analytical material models. This approach reduces the limitation of the virtual product model based planning as described above, since only the material property data of the constituent materials are required. Given the huge amount of possible composite micro- and meso-structure formations, that reduces the required physical characterization efforts enormously. It is important to mention that the freedom to virtually model the material structure at meso- and microscale allows for tailoring the material property values at continuum level and therefore provides means to directly analyze the impact on the product performance on macro- or part level. Following this cascade down to the molecular or even atomistic level would even further reduce the limitations of the virtual product model based planning, and the need for generation of experimental test data, respectively.

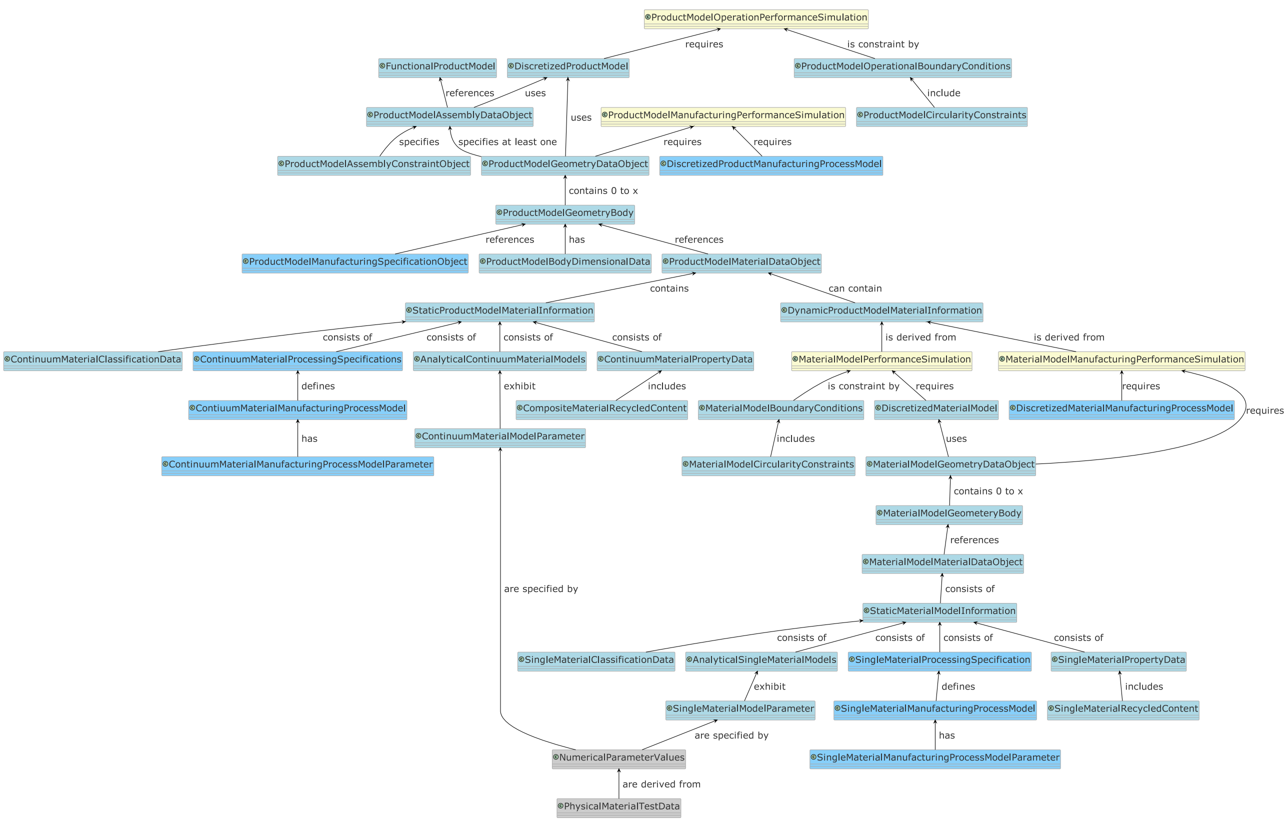


FIGURE 9 | Data model of multi-scale product model and design engineering chain. Color coding according to Figure 8, sky blue color indicates manufacturing related classes.

Apart from the material model and property data, the material data object can also contain information about process parameters for a qualified manufacturing process and the respective parameter values. Therefore, it provides the link to the manufacturability of the product or a specific composite material. Analogously to the virtually derived material property values, the material data object can also contain processing/synthesis specifications derived from a virtual processing/synthesis performance simulation (e.g., CALPHAD [36] or molecular dynamics on microscale) based on a discretized processing model. As the material data object exists on all scales, individual material manufacturability information, either experimentally or virtually specified, can also be referenced at each scale.

3.1.3 | *Product Operation and Circularity Model*

As product circularity requirements (unlike resource efficiency) are resulting from product performance with respect to reuse (or keeping in operation) repair, refurbish, remanufacture, and recycling (5R) [37] processes, we define circularity requirements to be a subset of the product operational requirements (see Figure 10).

That way, product operation naturally comprises multiple product lives and product material recovery, hence circularity. As the use of a product within a certain application can affect the physical product property values, its performance with regard to the 5R process requirements changes as well, eventually reducing the product's circularity potential to material recovery (recycling), closing the material cycle as the recovered materials can be consumed again in the product manufacturing processes. The product operation, including all 5R processes, can be understood as a process with defined process parameters consuming the physical product as input and providing it back with altered product properties. Therefore, the circularity potential or its suitability for a specific use or 5R process is always dependent on both, the specified process performance criteria and measures, as well as on the process induced changes in physical product properties. Since the circularity requirements are derived from specific 5R processes, any reasonable product circularity requirement specification should explicitly reference such processes in detail. With regard to the virtual product model, the product circularity requirements define the boundary conditions with respect to the product performance simulation.

3.1.4 | *Performance Model*

Unlike product and material properties, product and material performance can only be defined in reference to a process, a physical product or a product model is taking part in. Basically, performance describes how "well" a certain functionality is provided (in operation) under certain conditions and/or over a certain time. Hence, to determine, e.g., the product performance, first a performance expectation with respect to a specific product operation (process) needs to be defined. To quantify the performance expectation, this expectation has to be broken down into criteria, corresponding measures, and eventually specified quantities, which can then be compared to the actual values resulting from a measurement of these quantities, e.g., during the operation of a specific product. Hence, in the industrial or product context, the selection of characterization methods is driven by the definition of the performance expectation (see Section 3.2.4 for further details). It should be noted that a performance

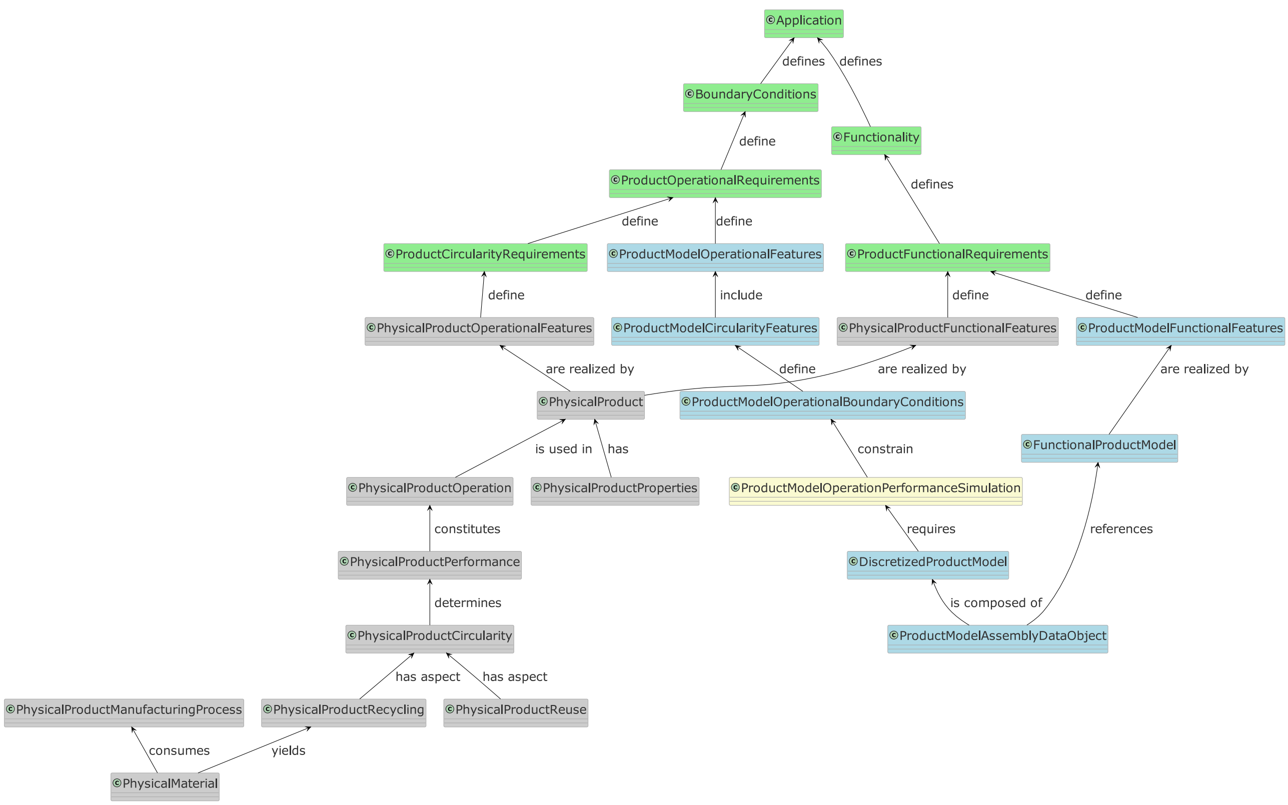


FIGURE 10 | Data model of product circularity. Color coding according to Figure 8.

quantification can also focus on the process itself. For example, if the performance (e.g., stability) of a certain manufacturing process needs to be determined, the process performance can be evaluated by characterizing changes/variations in the material property values of produced test specimen, consciously neglecting the resulting product performance in operation. The described model of performance and performance quantification applies to physical and virtual product models and their related processes (see Figure 11). In case of virtual product model performance quantification, the boundary conditions resulting from the operational requirements constrain the performance simulation (virtual measurement), e.g., deformation under load. As numerical simulation methods can only mimic the real physical interactions at different length scales to a limited extent, the performance assessment is still quite limited compared to the implementation of physical measurements.

3.1.5 | Combined Domain Data Model

Combining the individual data models discussed above based on their shared objects, one united domain data model was developed (see Figure A1 in Appendix A). It illustrates the cause-and-effect relationships as well as the interfaces between the individual domains and makes the prominent yet different roles of materials and processes for physical products and virtual product models transparent. It is worth noting that, even though developed to describe polymer matrix fiber reinforced composite materials and their related processes, the developed domain data model and its concepts shows generality beyond this specific example, making it ideally suited to expand into further domains related to industrial products and product life cycles.

3.2 | Domain Specific Models and Relation

Using the fiber reinforced polymers and their related processes as example and following the unified domain data model Figure A1 described above, detailed individual data models for the material related objects as well as the manufacturing, characterization, and simulation process related objects and their relations were developed. Regarding the process modeling, the variety of different processes required a uniform and standardized description, to facilitate the modeling process and the mapping to the ontology. Therefore, we tried to identify a process modeling framework that is on the one hand standardized or being standardized and on the other generic enough to model the wide range of physical and virtual processes. Additionally, we required the framework to provide the means to develop detailed, fine granular process descriptions as well as to be able to expand the modeling over the entire product life cycle. Based on these requirements, the VDI/VDE 3682 Formalized Process Description [38] (German: FPB) was selected. The basic structure of the FPB is illustrated in Figure 12. It establishes a clear separation between what a process does and how it is implemented. Each step of a process is described via a process operator that allows for three types of input and output objects, product, information, and energy. A system border defines which objects are entering the modeled process from the outside and which objects leave it again to the outside. The operator propagates the input objects from an initial state to next state. The operator can be composed and decomposed, which allows modeling on high level as well as very detailed level. Each operator has a technical resource associated, but does not depend on the technical resource itself (no machine model). The input objects as well as the process operator are very well aligned with the LCA methodology [39], which underlines the ability of the FPB to describe the entire product life cycle.

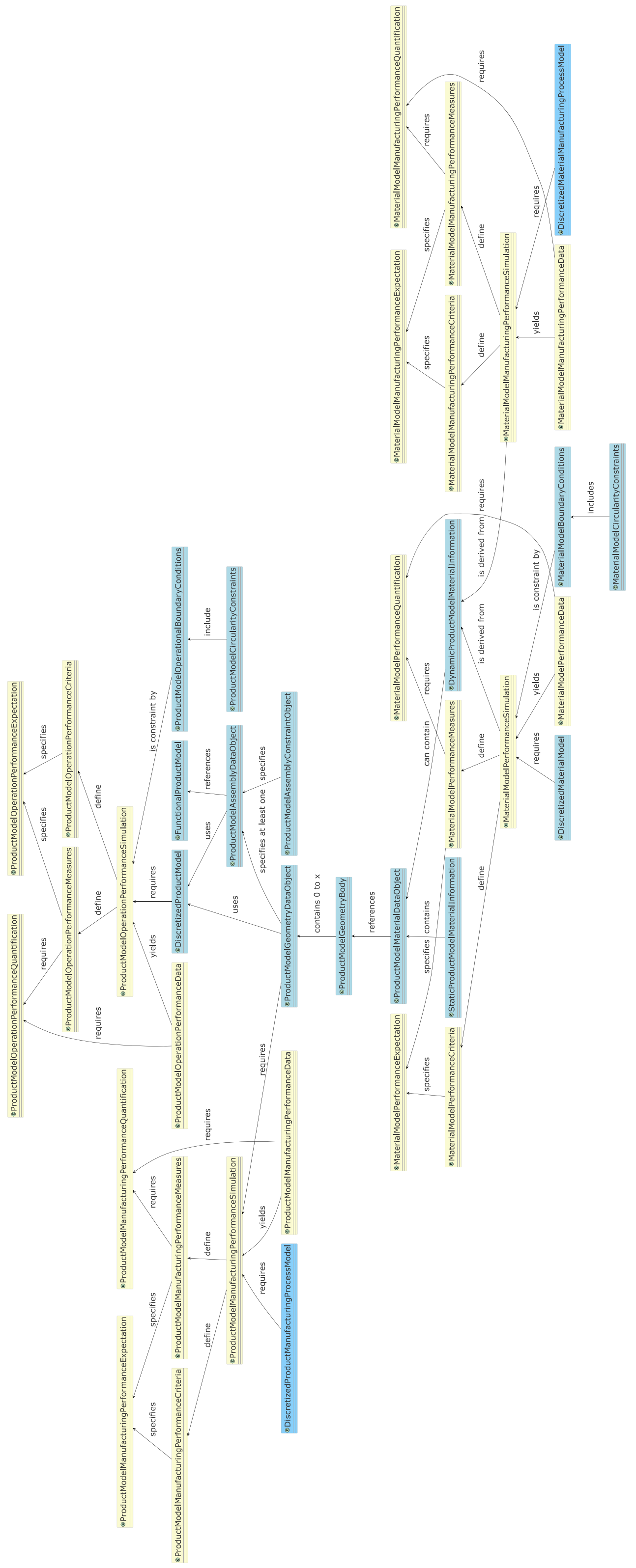
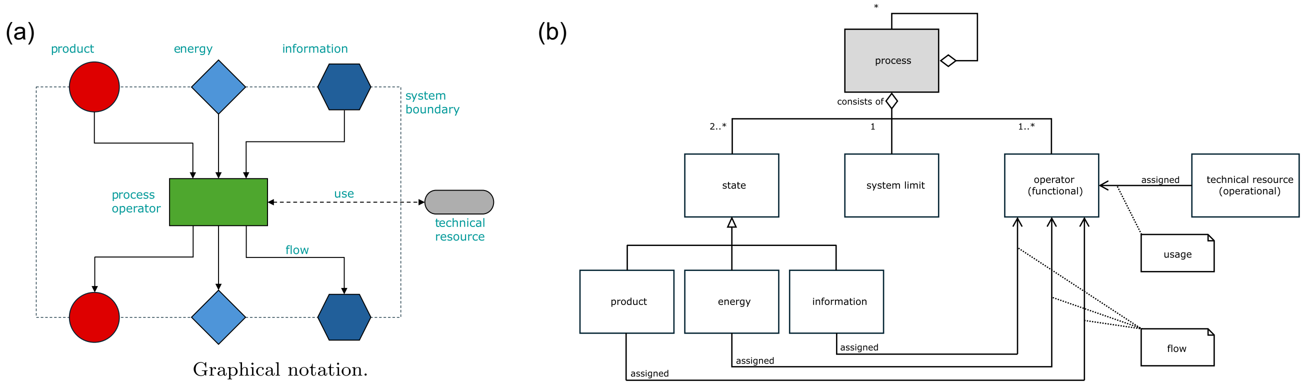


FIGURE 11 | Performance model on example of virtual multiscale product model. Color coding according to Figure 9.



Graphical notation.

Objects and relation (asterisk denotes integer number).

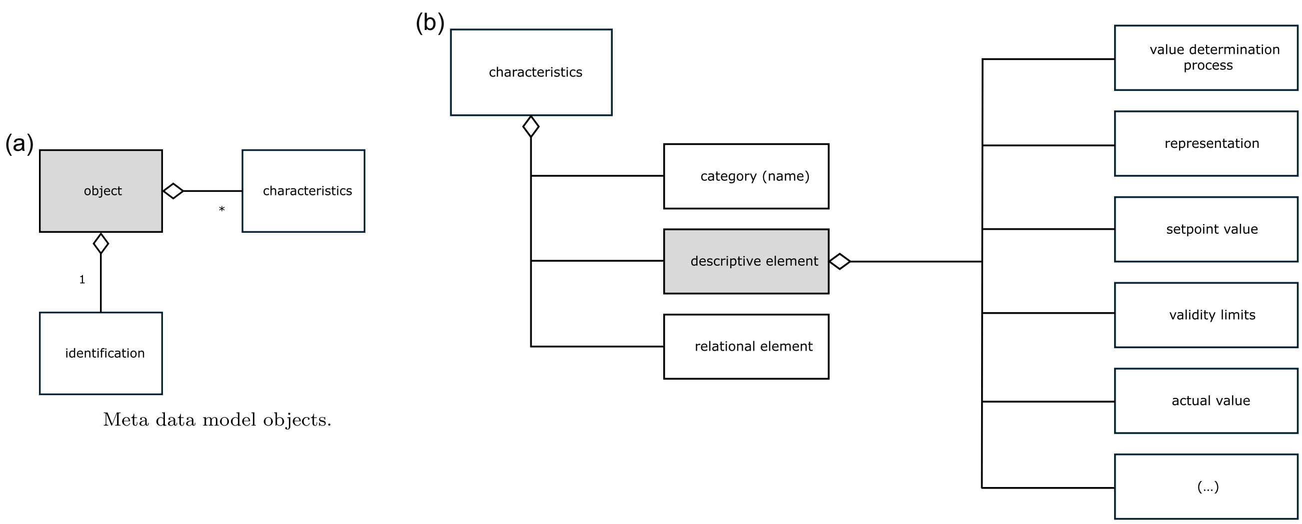
FIGURE 12 | (a) Notation and (b) objects of VDI/VDE 3682 process modeling framework.

The term product is a generic term that also represents the stream of materials, substances, etc. Each object has an unique identifier and attributes that describe the object in more detail and can also describe relations between objects; they are called descriptive and relational characteristics. Such characteristics can, for example, be process parameters or boundary conditions, which themselves can be further broken down, for example, into specified and as-is value characteristics (see Figure 13).

As the virtual product model (see Section 3.1.2) is considered a specification of the real product, we are using the freedom of the VDI 3682 process framework to also define the simulation models of components and materials as products, even though they do not physically exist. This allows us to model the physical and virtual world in full conjunction and to link the virtual and physical processes from characterization over fabrication, to operation, and end of life. The process modeling itself is carried out using the FPB Demo Tool (https://demo.fpbjs.net/) of Helmut Schmidt University, which provides (via an exportable .json file) the sequence, as well as all operators, information objects, products, and technical resources. In this way, process modeling in the FPB tool can be performed at the class level and in modules, without reducing the required level of detail (as detail can be provided separately, e.g., characteristics). The modeling of the process instances will be described elsewhere.

3.2.1 | *Multiscale Simulation Model*

For a more detailed numerical investigation of the mechanical properties of fiber reinforced polymers using FEM, the multiscale approach is particularly well suited. In this approach, a representative volume element (RVE) is first analyzed on the microscale. The homogenized mechanical properties obtained from this analysis are then transferred to the next higher scale level. The VDI/VDE 3682 formalized process description was used to develop a structured model of the multiscale simulation workflow. The challenge here lies in the fact that VDI/VDE 3682 was originally designed to model physical technical processes. However, during FEM simulation of materials at different scales, no physical object is actually processed and only data objects such as input files or solution files that do not exist in a conventional manufacturing process are generated. As we treat the simulated materials as representations of their physical counterparts, eventually specifying their properties (digital twins of materials), we model these data objects as (digital) products according to VDI 3682. Moreover, as the FE based simulation scheme adopted for the multiscale simulation incorporates a



Meta data model objects.

Meta data model characteristics (asterisk denotes integer number).

FIGURE 13 | Meta data model of VDI/VDE 3682 process modeling framework for (a) objects and (b) characteristics.

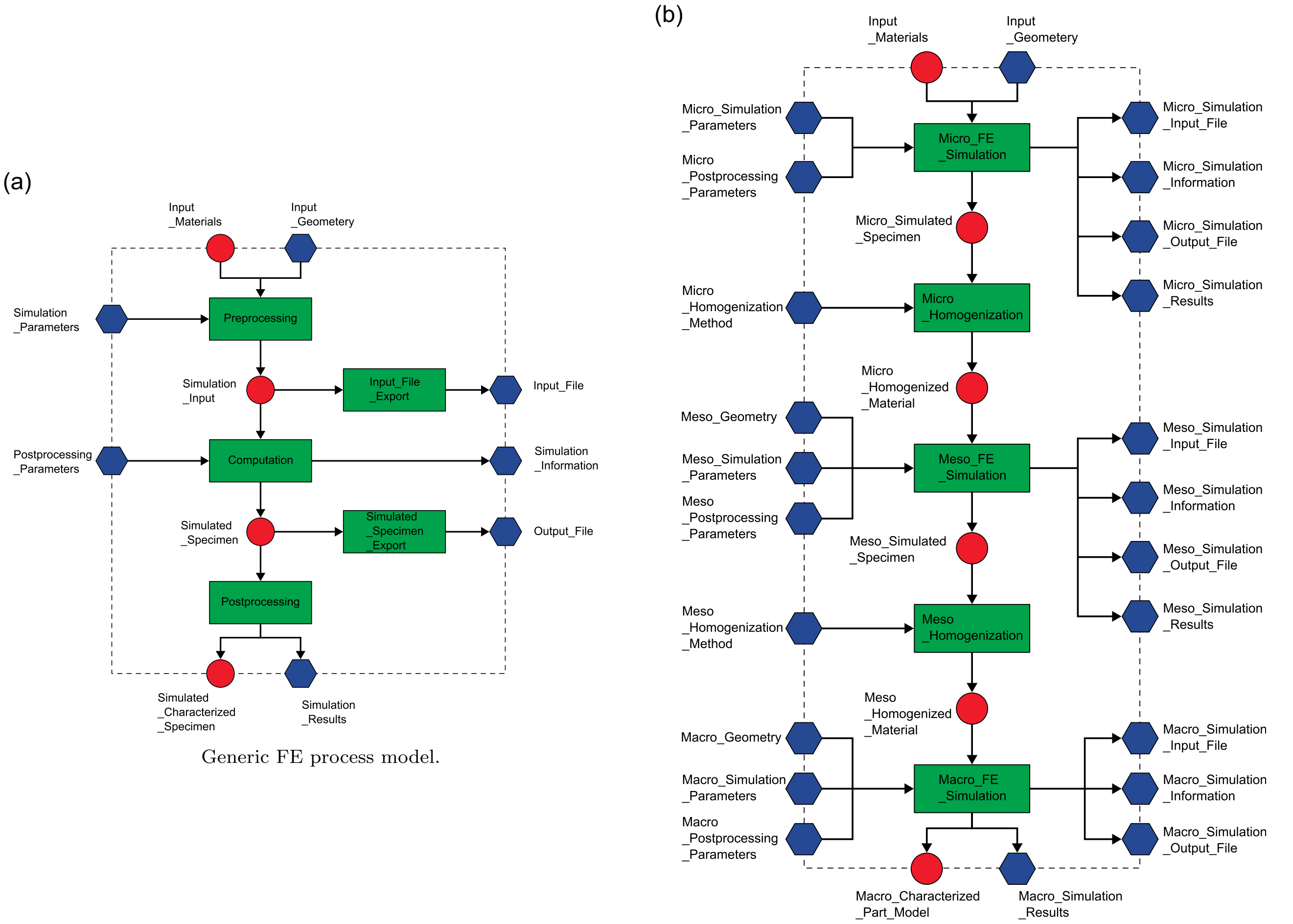
modular structure, we adopted this structure for the process model and developed a generic FE simulation model that can be applied to any single scale or within the multi-scale simulation process (see Figure 14a). The generic FEM simulation process module is divided into the main operators preprocessing, computation, and postprocessing. The digital material is passed through all these operators, with each operator modifying the digital material. Analogous to real processes, the preprocessor processes the *raw* digital material in the form of numerical material parameters together with geometric and other boundary conditions to create a simulatable material. This is then processed into a simulated material during the calculation step. The post-process completes the simulation process by processing the simulated material or simulated specimen into a simulated and characterized material. The intermediate material states may be exported optionally for user investigation through additional operators.

The multiscale simulation process is an excellent example for the modularity of the VDI 3682 standard, as can be seen in Figure 14b. Here, the generic FE simulation process is reused sequentially for each scale. This modular structure is a key element of the simulation workflow, enabling a fast and efficient setup of new multi-scale simulations.

In the given process, the multi-scale simulation consists of three different scales: the micro-, meso-, and macro-scale. After the micro- and meso-scale is the homogenization operator, which extracts the homogenized material properties from the simulated materials by evaluating the stresses and strains on the RVE boundaries. Thereby, the effective stress-strain relationship of each scale are deduced, which includes the potentially 21 independent stiffness components. The homogenization operator is a special case of a postprocess. Hence, it was modeled as a separate operator after the generic postprocess, since not every FE simulation concludes with a homogenization.

3.2.2 | MEX Process Simulation Model

The MEX process simulation model, created according to VDI 3682, uses the generic FE simulation module template as described above (Section 3.2.1). The process simulation has two separate simulation steps that interact with each other. The whole model is shown in Figure 15. The information objects on the left side of the system border specify the parameters that define the boundary conditions and output options of the simulation operators. They provide details on the step-size configuration of the simulation, the chosen FE elements, the G-Code from the printing process, etc. Since they differ for the mechanical and thermal simulation, they are doubled and not shared between the simulation process operators. The material properties are defined in the corresponding product at the top, analogously to the multi-scale simulation. The information objects on the right side of the system



Generic FE process model.

Multi-scale simulation process model.

FIGURE 14 | FE simulation process models: (a) generic and (b) multiscale based on VDI/VDE 3682.

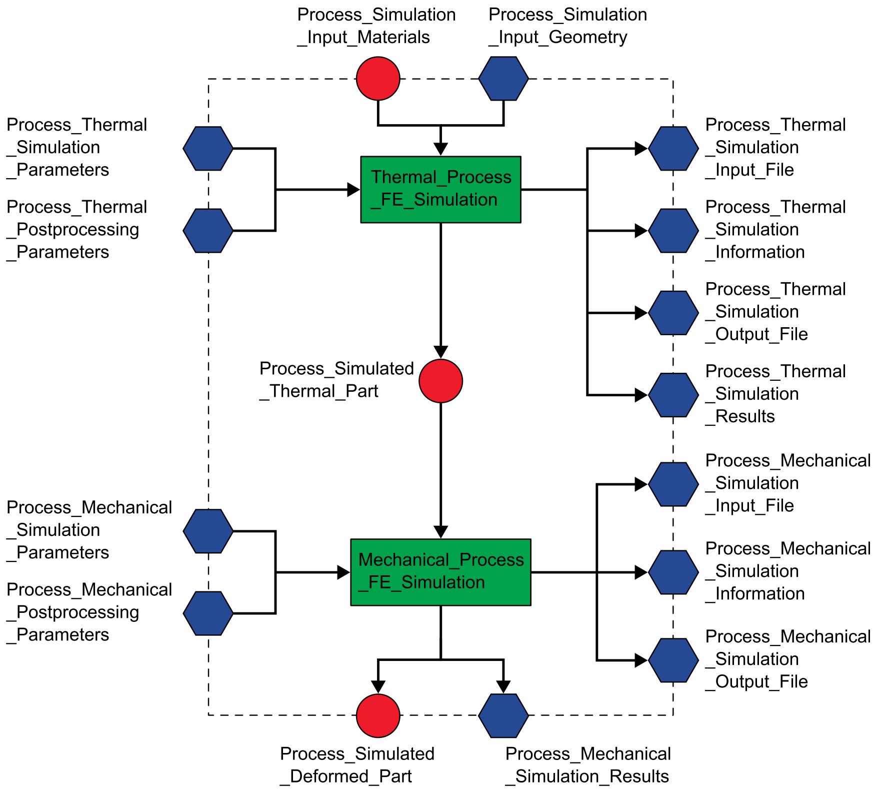


FIGURE 15 | MEX process simulation model based on VDI/VDE 3682.

boundary contain the simulation results. The input file is also saved since it contains all information from the performed simulation. This approach allows for the traceability and reproducibility of simulations while avoiding the need to store all data individually and prevents the loss of simulation parameters. The output operators are divided into the simulated part and the simulation results to differentiate between the simulated part with the resulting information for every element and every time step on the geometry and selected simulation results that are provided depending on the specific research question. For example, when a 3D printing process is thermally simulated, the temperatures occurring during the process are computed based on the applied thermal boundary conditions and material properties. The simulated part product then contains temperature information for each element at every time step. In contrast, the ThermalSimulationResult information object would contain, for instance, three temperature-time histories represented as value pairs for three representative points of the component. The thermal simulated part is then used as a input for the thermal simulation. The temperatures from the thermal simulation are mapped on the structural mesh and the resulting thermal strains and stresses are computed. The results are analogous stored in a deformed part and simulation results information object at the bottom of the system boundary.

3.2.3 | *Manufacturing Process Models*

3.2.3.1 | MEX Process Model. The model of the physical Material Extrusion (MEX) process, according to VDI 3682, is primarily structured around the material flow, which is illustrated in the Appendix A due to size reasons in Figure A3. The thermoplastic material is—in this order—dried, conveyed, fed into the extruder, plastified by the combined action of thermal energy and shear, extruded through the nozzle, and deposited along a defined path. Subsequent cooling and solidification of the deposited strands result in the formation of the final component. In addition to the material flow, the process comprises a set of supporting and control operations that are essential for stable and reproducible manufacturing. The slicing operation, while representing a preparatory step, provides the digital process description and thus forms the basis of the continuous control operation. During process execution, this control operation supplies setpoints and commands to subordinate operations, including thermal control, mechanical actuation, and kinematic positioning of the extruder system. Furthermore, peripheral subsystems such as the heated build chamber and the build platform are operated and regulated based on the information generated within the control operation, ensuring consistent process conditions throughout the manufacturing sequence.

3.2.3.2 | Injection Molding Process Model. The model of the injection molding process according to VDI 3682 describes the injection molding process to generate a part made of short or long fiber reinforced thermoplastics. The schematic representation of the process is shown in Figure 16. The incoming product that is used for this process is usually provided in form of granules that contains thermoplastic resin and chopped fibers and fillers. In a first process step, this incoming material is conveyed and dosed to the plasticizing unit. There, the material is melted and mixed. The plastified mixed thermoplastic material is then injected into a mold with a specific temperature. In the mold, the melted material is packed and formed into desired shape. In addition, it is cooled down to ejection temperature. The ejection process step is executed by the ejector unit. Afterward, the warm ejected raw product is transported to the finishing unit where it is cut

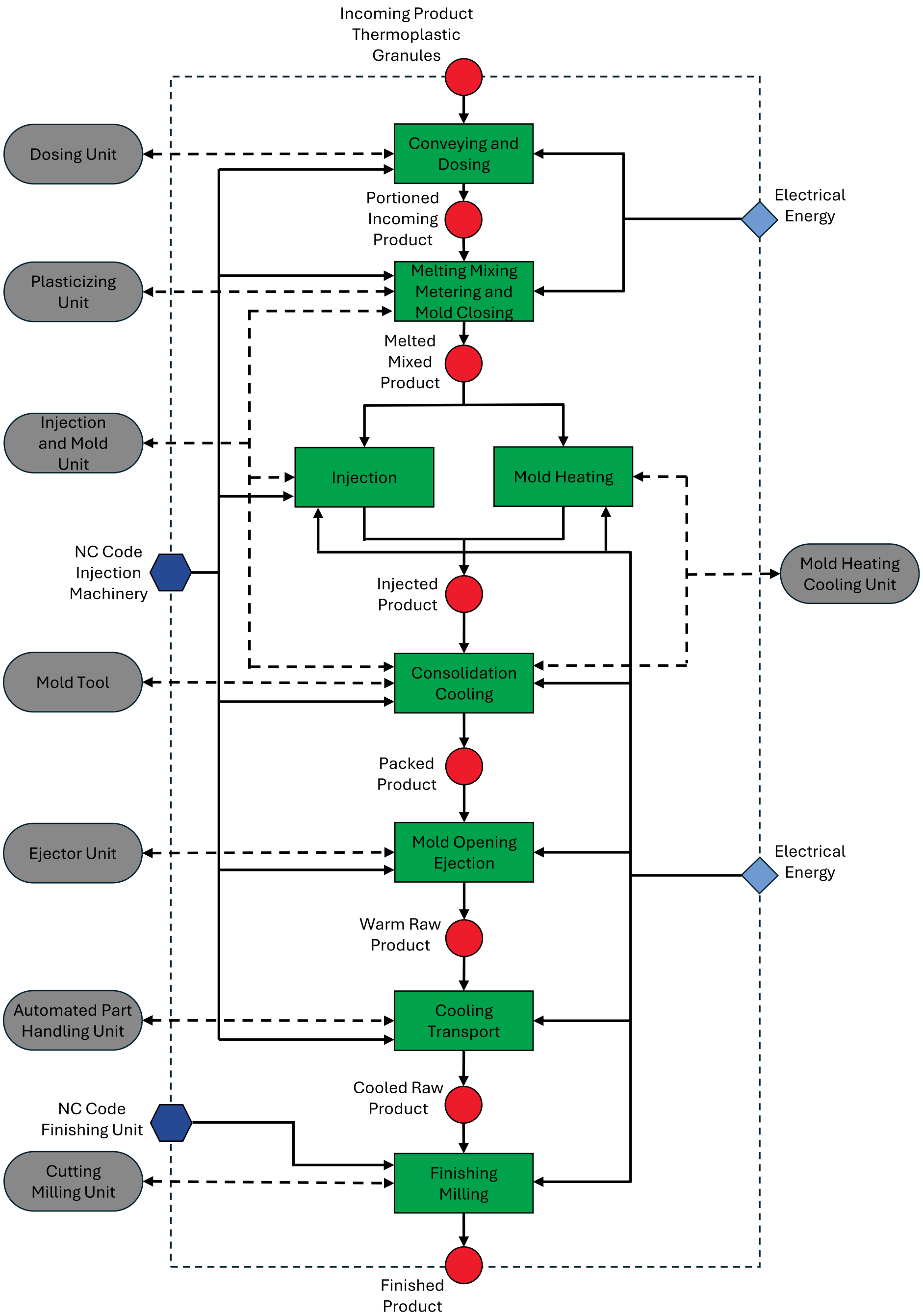
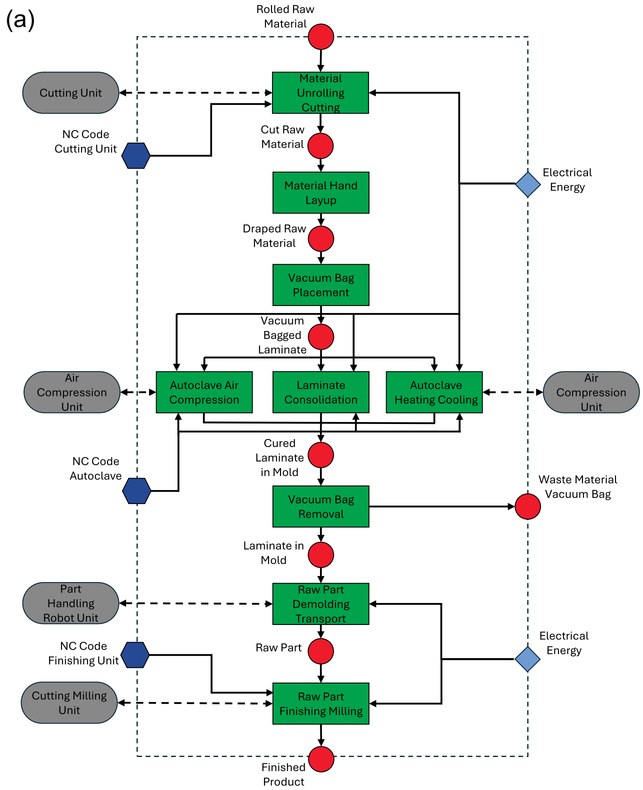


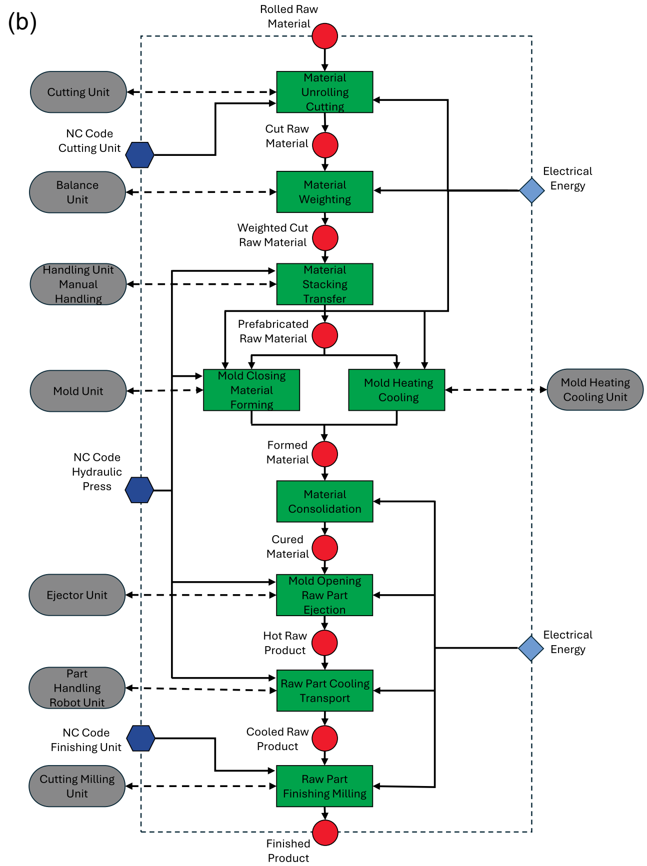
FIGURE 16 | Injection molding process model based on VDI/VDE 3682.

and milled if necessary. During transportation to the cutting and milling unit the warm raw product is cooled down. After this process step, the final finished product can be removed from the cutting and milling machine. All the movements of the machinery and process conditions during the injection molding and finishing process are controlled by NC code.

3.2.3.3 | *Compression/Autoclave Molding Process Model.* The autoclave and compression molding processes are fundamentally very similar and are therefore dealt with together in this section. The model of the autoclave process according to VDI 3682 is shown in Figure 17a and the compression molding process in Figure 17b. The autoclave process begins with a rolled preimpregnated raw material ('prepreg'). In a first step, the material is unrolled and cut. The pieces of cut prepreg material a stacked depending on the desired number of layers and then placed into a vacuum bag. The stacked layers of prepregs is called a laminate. In the next process step, the vacuum bagged laminate is placed in the autoclave where three processes are running simultaneously. That are the autoclave air compression to compress the laminate and push out voids, the autoclave heating and later cooling and the process of resin consolidation. The controlled sequence of these processes is referred to as an autoclave cure cycle. After the consolidation of the material, the vacuum bag is removed, and the laminate is demolded. The raw part laminate is then transported to the finishing unit where milling operations are performed to create the final shape of the part. In contrast to the autoclave process, bulk materials such as bulk molding



Autoclave process model.



Compression molding process model.

FIGURE 17 | (a) Autoclave and (b) compression molding process models based on VDI/VDE 3682.

compounds (BMC) and sheet molding compounds (SMC) are mainly used for compression molding. The raw material is cut, weighted, and then stacked. An important difference between the autoclave and the compression molding process is that for the latter process, there is no vacuum bag used. Instead, the stacked material is placed directly into a mold. In the next process step, the mold is closed and applies a very clamping force to the material which is formed during that step. The mold is heated up in this process by a heating and cooling unit. The formed material is then cured in the heated mold. If required, there can be a cooling phase processed by the heating and cooling unit. After the material is fully consolidated, the mold opens, and the hot raw part is ejected by the ejector unit. The next process steps are similar to those in the autoclave process. The raw part is cooled and transported to the finishing unit.

3.2.3.4 | *Resin Transfer Molding Process Model.* The model of the resin transfer molding process according to VDI 3682 is shown in Figure 18. This process begins with two incoming products, which are a fiber fabric and a liquid epoxy resin. The fiber fabric is cut into cut and then stacked and draped into a mold. Afterward, the mold is closed and heated by a mold heating unit. At the same time, the epoxy resin is compressed in a pressure vessel. The pressure vessel has a connection to the mold that is closed at the beginning. When the mold closing and heating process is completed, the valve is opened, and the compressed liquid epoxy resin is injected into the mold. During injection, the resin infiltrates the fiber fabric. This process can be vacuum assisted. At the end of this process step, a fully impregnated mixed product is generated which consists of fibers and epoxy. Now, the epoxy resin cures under controlled temperature. After the resin has completely cured, the mold is opened, and the hot raw product is ejected by the ejector unit. During transportation, the hot raw product is cooled down. The final step is the finishing milling which puts the composite into its desired shape.

3.2.4 | *Characterization Process Model*

The model of the characterization processes, according to VDI 3682, separates into a planning and the actual characterization process (see Figure 19). This reflects the application of characterization and test processes in the industrial context and allowed for a generic, characterization method independent process model. The planning process (see Figure 19a) precedes the actual physical characterization process. It models how information about available metrology techniques, product, or process performance expectation is used to select a specific metrology technique and to define the physical quantities that will be measured once the characterization process is implemented. At the same time, the respective parameter space of the metrology technique and the calibration information are derived. After concluding the planning process, the resulting output information objects are input to the physical characterization process (see Figure 19b).

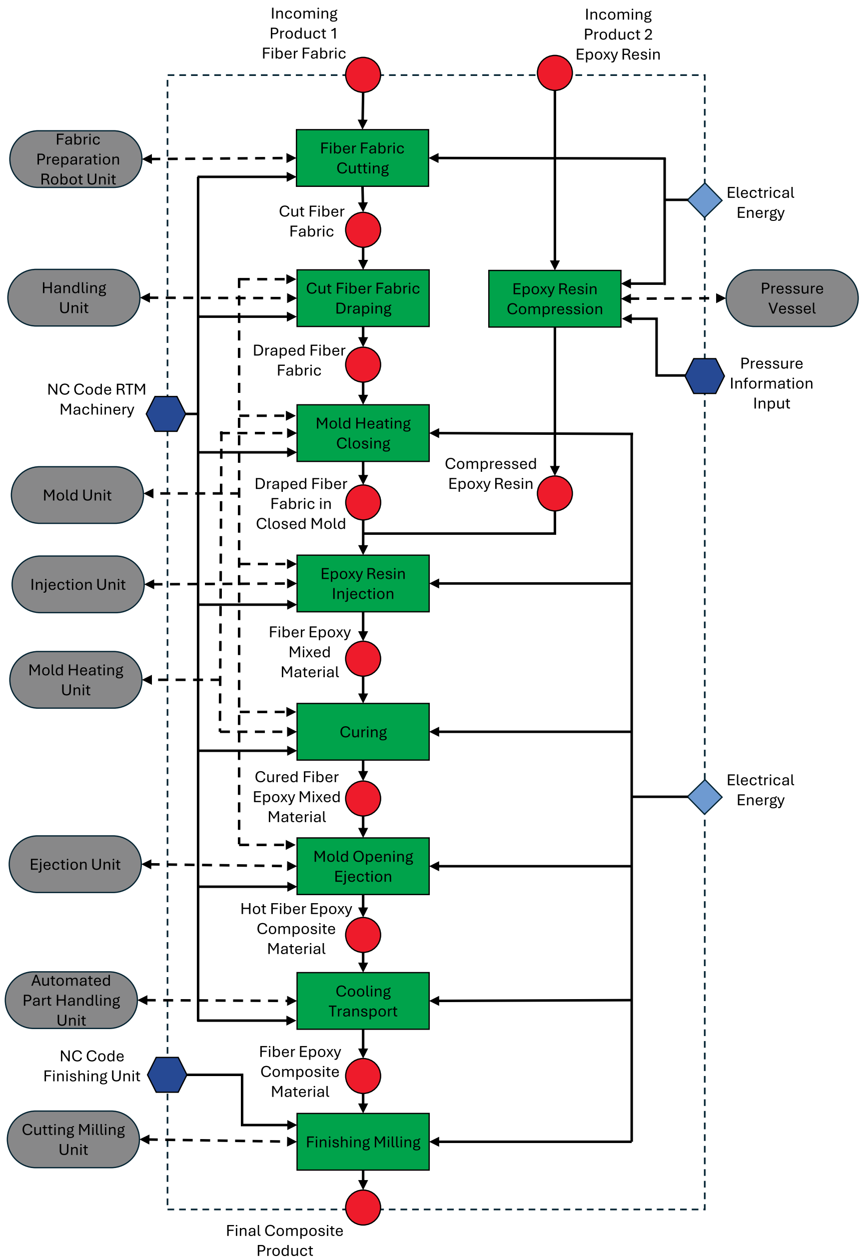


FIGURE 18 | Resin transfer molding process model based on VDI/VDE 3682.

The process model shows how a physical object under consideration is characterized based on a predefined measurement technology and how its performance with respect to the predefined physical quantities is derived. The physical characterization process acts as the central process operator, to which the physical object is fed as a product. Furthermore, information-based input variables such as the calibration properties of the measurement technology and selected measurement parameters are incorporated into the process. The technical resource "measuring equipment" is assigned to the process operator and represents the necessary infrastructural prerequisite for performing the measurement. The actual measurement generates measurement data, which is transferred as an information flow to downstream data processing. In this step, the raw data is processed and converted into descriptive data. This is followed by performance quantification, in which object-related performance indicators are derived from the determined physical quantities and the processed measurement data. The result of the overall process is, on the one hand, a characterized physical product and, on the other hand, a structured amount of information in the form of quantified object performance.

As the model provides a generalized description of the physical characterization process, specific implementations of the process with different metrology methods can be described as various instances of this process. Consequently, the three testing and characterization methods defined in OntOMat

- Digital holography
- X-ray computed tomography
- Mechanical tensile/conventional testing

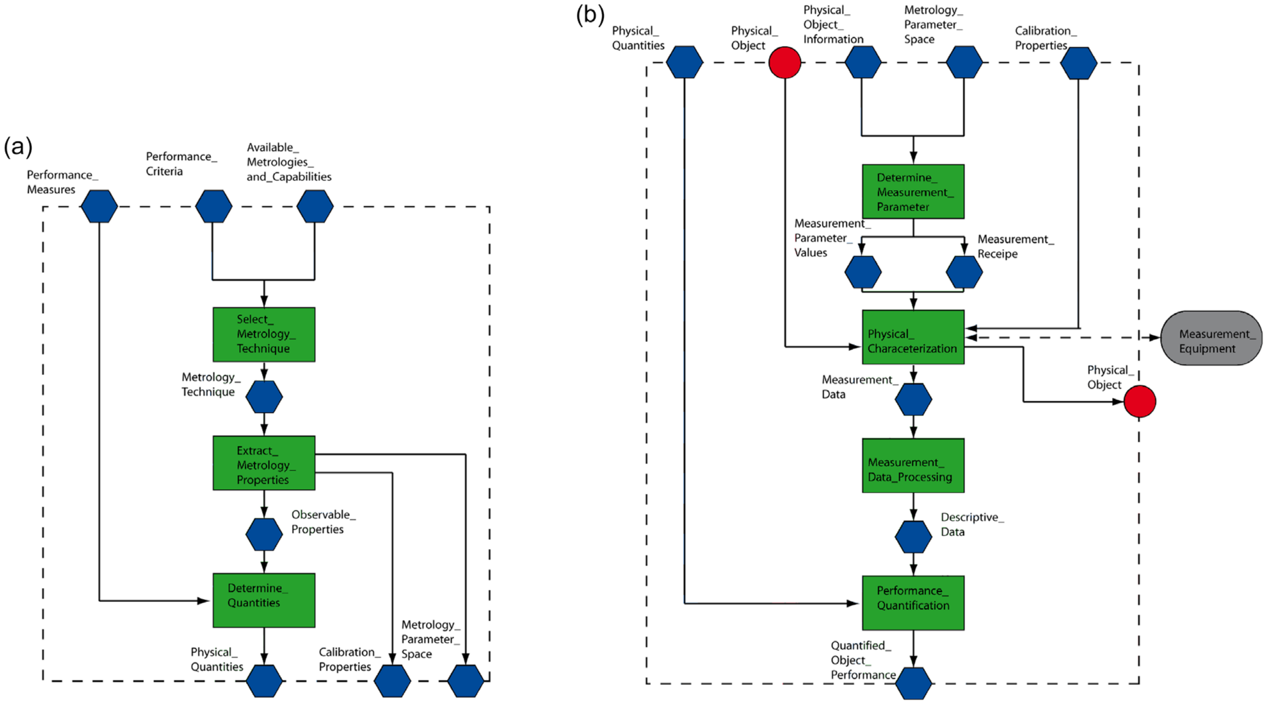


FIGURE 19 | (a) Planning process model preceding the physical characterization process based on VDI/VDE 3682. (b) Generic physical characterization process model based on VDI/VDE 3682.

can be represented purely by specifying the method-specific parameters.

3.2.5 | *Stochastic Process Model*

In general, the experimental or numerical characterization of material properties is not carried out in a single experiment or simulation, but requires repeated execution of the experiment or simulation in order to determine the scatter and the probability of occurrence of the property of interest. Every deterministic process, whether physical or digital, can be embedded into a surrounding stochastic process. This allows the deterministic process to be repeated arbitrarily often and statistical moments of relevant quantities to be obtained, for example, the statistical mean and the standard deviation. Within the framework of VDI 3682, our approach is represented by the process model shown in Figure 20.

Here, we assume that both physical and digital processes are deterministic, i.e., that identical input yields identical output. The statistical scatter observed when processes are repeated can be explained by variations in the inputs, which also include boundary conditions such as environmental conditions.

The stochastic process comprises both the deterministic specimen manufacturing process and the deterministic characterization. In this context, the term “specimen” may relate to the physical, i.e., laboratory specimen or the numerical model used in a multiscale simulation. In addition to the conventional inputs required for manufacturing and characterization, namely the raw material and the respective process information, the key input is the information object describing the stochastic parameters. This information object contains, among other things, details on the stochastic model, the number of repetitions, and the methodology used to select the individual specimens. The stochastic model specifies, for example, how the specimens are distributed (e.g., normally or log-normally distributed). Consequently, this information also feeds into the specimen manufacturing process to ensure that an appropriate sample of test specimens can be produced.

After the manufacture or generation of the required specimens, implicitly including digital twins, an iteration over the deterministic characterization process is performed. This is realized by means of the iterator operator and a counting variable i. Using the selector operator, a specimen is passed to the deterministic virtual or laboratory characterization process based on the value of i. Taking into account the process information additionally provided, the process is executed and the results are passed to the stochastic post-processing operator. In parallel, the iterator operator compares the counting variable $i$with the required number of repetitions n to decide whether another specimen is to be passed to the deterministic process or whether the desired number of repetitions has been reached. In the latter case, the stochastic post-processing operator evaluates the individual results and outputs the desired statistical moments. The possible outputs of the iterator operator represent alternative paths and therefore never occur simultaneously.

A specific challenge in modeling the stochastic process within VDI 3682 is the representation of iterative loops with a variable number of repetitions. The VDI 3682 standard defines process operators that transform input states into output states via directed flows. However, it does not provide explicit formal constructs for iteration, such as loop termination conditions, counting variables, or convergence criteria. While the standard does not strictly prohibit cyclic connections, i.e., an output state of a downstream operator may, in principle, serve as input to an upstream operator, its graphical notation, accompanying examples, and the available modeling tool (FPB Demo Tool) are

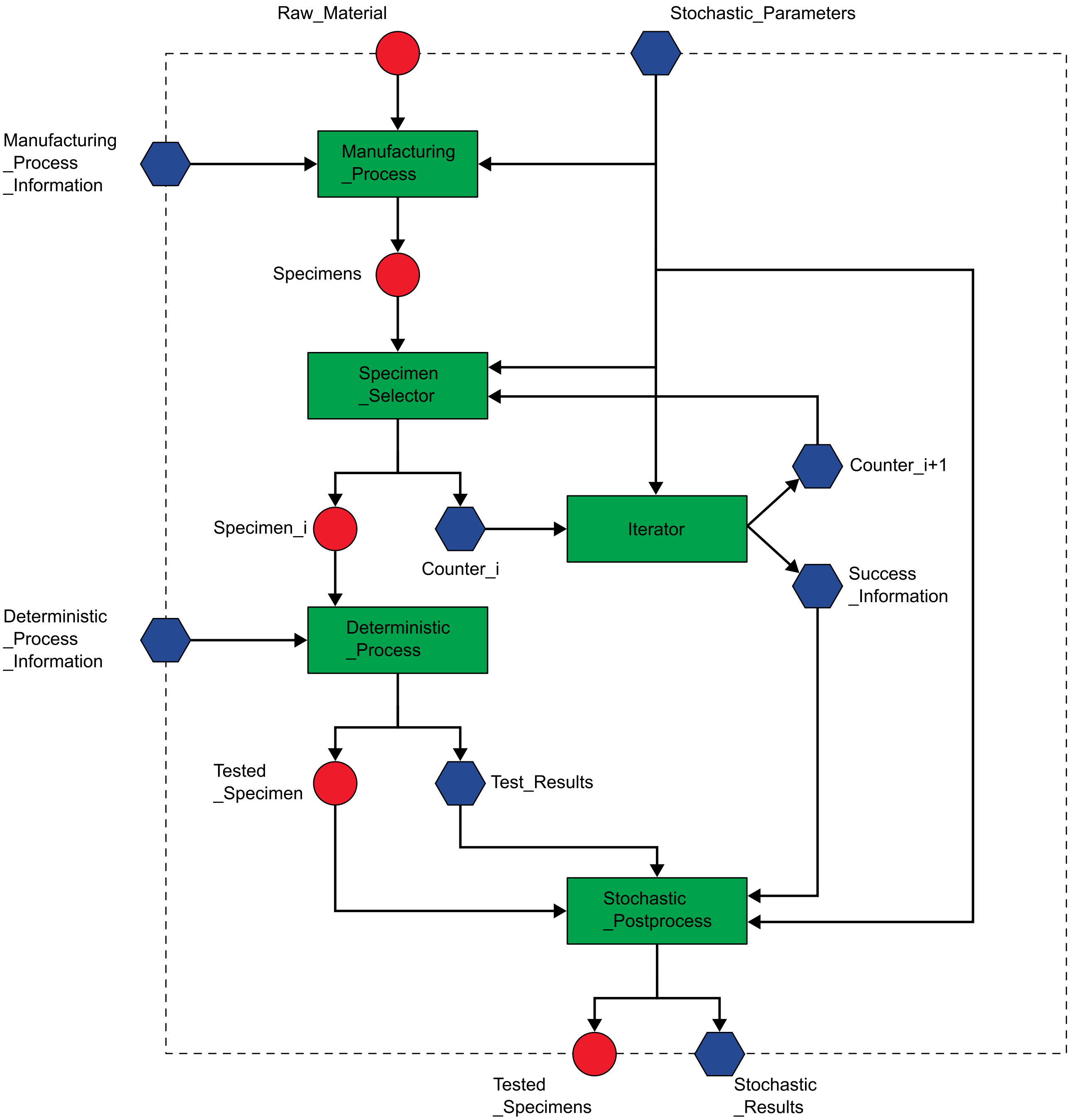


FIGURE 20 | Stochastic process model based on VDI/VDE 3682.

designed primarily for linear, feed-forward process descriptions. In the FPB Demo Tool, connections from downstream to upstream operators cannot be drawn directly. This tooling constraint was circumvented by first placing the target operator downstream of the source operator, establishing the connection, and subsequently repositioning the target operator to its intended upstream location, thereby preserving the connection. The resulting process model (Figure 20) thus represents the iterative loop as a cyclic flow within the VDI 3682 operator graph.

3.2.6 | Material Model

The general understanding of materials, building the base for the entire modeling concept, is summarized below:

Subset/category of matter differentiated(under defined conditions) by specific intensive quantifiable physical and chemical properties (quantities) and/or their respective values (commonly referred to as material properties and property values).

Further, the material modeling concept is driven by the hierarchical structure of the fiber reinforced polymer composite materials giving rise to **multiscale modeling** and morphologic material properties. Additionally, a clear separation between **material properties**, which are generally applicable, and material **property values** is made. As materials are always considered in conjunction with their processing, the material property values are assumed to be **constantly evolving** during the life cycle of the material (and/or product) from first synthesis, over processing, to its altering during the respective product operation. Moreover, a clear distinction between materials or rather material instances created by processes outside of the modeled domain (for which the material instances are not physically available), and the materials resulting from the processes modeled within the domain for which the material instances are physically available, is made. The first category is in the following referred to as "nominal materials." The concept of nominal materials was introduced to clearly emphasize that the corresponding property values do not possess universal validity and are merely to be understood as an approximation of the real property values of material instances. To comprehensively model the (nominal) polymer matrix fiber-reinforced composites according to above definitions, a template, in the following called "nominal material template," was developed (see Figure A2 in Appendix A). Besides the material modeling aspect, this template forms the basis for the mapping to the developed ontology (see Section 4).

The hierarchical structure of the fiber-reinforced polymer matrix composites is modeled via the breakdown of the composite into its constituents and the interphase between reinforcement and the polymer matrix. Hence, each composite material model at least consists of two constituents and one interphase. Constituents and interfaces are modeled with the same modeling scheme as the composite material itself, meaning the same attributes are used to describe the composite as a whole as well as the individual constituents. Treating the interphase as individual material, even though being an oversimplification, is motivated by drastically different material property values determined for the interface region. As the interface region is modeled as individual geometric region of the RVEs (see Section 2.2.3), the assignment of specific interphase properties as part of the virtual material model becomes feasible. As the physical material is understood as a subset of matter, the material properties are generally applicable attributes that can be used to describe a specific material. Hence, a unified set of intensive material properties relevant to fiber-reinforced polymer matrix composites, ranging from mechanical, thermal, over chemical, to optical properties was defined and automatically applied to the modeling of the nominal composite materials as well as their constituents. To allow for the detailed modeling and quantitative description of the material microstructure, additionally, a set of generally applicable morphological material properties was defined and applied (see Section 2 and Table 2).

If a certain property is not quantified via a measurement/characterization, the property is still carried forward or assumed to be inherited to a specific material instance and therefore quantifiable whenever desired. Since fiber-reinforced polymer composite materials usually exhibit an anisotropic micro-structure, the material properties in the different Cartesian directions are based on the local fiber orientation and length distributions. This includes elastic and strength properties, but also, for example, thermal conduction. Since spatial directions cannot be defined independently of the observer, we introduce a Cartesian coordinate system as the basis for anisotropic properties of the material, which is materially oriented to the elastic properties of the product. The first spatial direction x_1 is chosen so that it coincides with a direction of maximum stiffness. Orthogonal to this, the second spatial direction x_2 corresponds to a maximum stiffness direction in the normal plane to x_1 and the third spatial direction x_3 completes the orthonormal system. The choice of such a coordinate system is never unambiguous, as immediately becomes clear when considering an isotropic material. The advantage of choosing this coordinate system is that material symmetries frequently occurring in FRPs, such as transverse isotropy, are directly recognizable in the stiffness components. The so defined material properties are equally applicable to the physical test specimen and samples as well as the virtually simulated materials (material twins). To account for the stochastic nature of all physical or their virtual processes (see Section 1), each material property value is required to be described as mean value including the standard deviation. If the standard deviation is set to 0, it is assumed that no statistical evaluation was performed or is available. Furthermore, the nominal material property values are enriched with several attributes providing provenance information, e.g., the test standard or test environment used, or the data source, e.g., if originating from a data sheet or publication. In addition, a set of typical material and/or semi-finished product forms was defined for the specification of extensive material properties. To further increase standardization and generalization, material classes according to IEC 62474 were adopted and adapted to account for the specific characteristics of polymer matrix fiber-reinforced composites. In this context, the existing material classes were extended by "Fiber Reinforced" and "Thermoset Filled," and missing material classes were added. As data generation and provision follow the FAIR principles (Findable, Accessible, Interoperable, and Reusable), the modeling and storage of metadata and provenance information play a crucial role. The consortium therefore agreed on the use of the PROV-O upper ontology (https://www.w3.org/TR/prov-o/) and incorporated the corresponding data fields into the nominal material template. All units of the property values are described based on the QUDT ontology (https://www.qudt.org/) to make them automatically convertible inside the knowledge graph.

3.2.7 | *Material and Process Relation Model*

Figure 21 illustrates the relation between the process modeling according to VDI 3682 and the developed material model giving rise to the developed nominal material template (see above). As physical products are physical objects that embody matter, each physical product will have an associated material instance that will be specified by the intensive physical material property values resulting from the underlying physical processes.

3.3 | Competency Questions

As part of the ontology requirement engineering process, competency questions were formulated. The competency questions can be clustered into five main categories:

- (Virtual) process engineering
- Manufacturing process and equipment
- Material/product characterization
- Physical product production and traceability
- Virtual product design/engineering

Table 3 shows a selected set of competency questions within each category.

TABLE 2 | Unified set of intensive material properties grouped by property super class. Properties marked with (∗) are derivable from other entries.

Property class	Components	Symbol	Unit
Mechanical physical properties			
Density	—	ρ	kg/m^3
Nominal weight	—	w	g/m^2
Geometrical properties			
Surface roughness	—	R_a	μm
Viscosity	—	μ	Pa s
Dynamic viscosity	—	η	Pa s
Kinematic viscosity*	—	ν	m^2/s
Thermal physical properties			
Glass transition temperature	—	T_g	K
Melting point	—	Θ	K
Heat deflection temperature	—	HDT	°C
Thermal conductivity	—	λ	W/(m K)
Heat transfer coefficient	—	h	$W/(m^2\ K)$
Thermal expansion coefficient	3	$\alpha_{11}, \alpha_{22}, \alpha_{33}$	$10^{-6}\ K^{-1}$
Specific heat capacity	—	c	J/(kg K)
Water absorption	—	—	wt%
Optical properties			
Refractive index (ordinary)	—	n_o	—
Refractive index (extraordinary)	—	n_e	—
Transmission coefficient	—	T	—
Absorption coefficient	—	α	—
Reflection coefficient	—	R	—
Elastic properties			
Symmetry class	—	Sym	—
Stiffness matrix	21	C_{ij}	GPa
Compliance matrix*	21	S_{ij}	GPa^{-1}
Elastic modulus*	3	E_1, E_2, E_3	GPa
Shear modulus*	3	G_{12}, G_{13}, G_{23}	GPa
Tensile modulus	3	$E_1^{tens}, E_2^{tens}, E_3^{tens}$	GPa
Flexural modulus	3	$E_1^{flex}, E_2^{flex}, E_3^{flex}$	GPa
Compression modulus	3	$E_1^{comp}, E_2^{comp}, E_3^{comp}$	GPa
Poisson's ratio*	3	$\nu_{12}, \nu_{13}, \nu_{23}$	—
Strength properties			
Tensile strength	3	$R_{m,1}, R_{m,2}, R_{m,3}$	MPa
Strain at tensile strength	3	$\varepsilon_{u,1}, \varepsilon_{u,2}, \varepsilon_{u,3}$	MPa
Tensile stress at fracture	3	$\sigma_{f,1}, \sigma_{f,2}, \sigma_{f,3}$	MPa
Tensile strain at fracture	3	$\varepsilon_{f,1}, \varepsilon_{f,2}, \varepsilon_{f,3}$	MPa
Compression strength	3	$R_{m,1}^{comp}, R_{m,1}^{comp}, R_{m,3}^{comp}$	MPa
Compression stress at fracture	3	$\sigma_{f,1}^{comp}, \sigma_{f,2}^{comp}, \sigma_{f,3}^{comp}$	MPa
Flexural strength	3	$R_{m,1}^{flex}, R_{m,2}^{flex}, R_{m,3}^{flex}$	MPa
Yield strength	3	$R_{e,1}, R_{e,2}, R_{e,3}$	MPa
Shear strength	3	$\tau_{S,12}, \tau_{S,23}, \tau_{S,13}$	MPa
Interfacial shear strength	3	$\tau_{IFSS,12}, \tau_{IFSS,13}, \tau_{IFSS,23}$	MPa

(Continues)

TABLE 2 | (Continued)

Property class	Components	Symbol	Unit
Interlaminar shear strength	3	$\tau_{ILSS,12}$, $\tau_{ILSS,13}$, $\tau_{ILSS,23}$	MPa
Flow stress	3	$Y_{f,1}$, $Y_{f,2}$, $Y_{f,3}$	MPa
Morphological properties			
Bio-degradable material content (mass)	—	$w_{bio-deg}$	%
Bio-feedstock material content (mass)	—	$w_{bio-feed}$	%
Recycled material content (mass)	—	w_{rec}	%
Matrix material content (mass)	—	w_{matrix}	%
Fiber material content (mass)	—	w_{fiber}	%
Particle material content (mass)	—	$w_{particle}$	%
Matrix material content (volume)*	—	v_{matrix}	%
Fiber material content (volume)*	—	v_{fiber}	%
Particle material content (volume)*	—	$v_{particle}$	%
Avg. particle/pore distribution	—	—	m^{-3}
Avg. particle/pore size	—	—	m^3
Avg. particle/pore shape†	—	—	%
Avg. particle/pore orientation	—	—	°
Avg. particle/pore composition	—	—	%
Avg. fiber length	—	l_{mean}	μm
Avg. fiber diameter	—	d_{mean}	μm
Avg. filament semi-minor axis	—	—	μm
Avg. filament semi-major axis	—	—	μm
Avg. yarn fraction (mass)	—	—	%
Fiber orientation tensor	5	A_{11}, A_{22}, A_{12}, A_{13}, A_{23}	—

*Derivable from other listed properties (retained for practical convenience).
†Shape deviation to enclosing sphere.

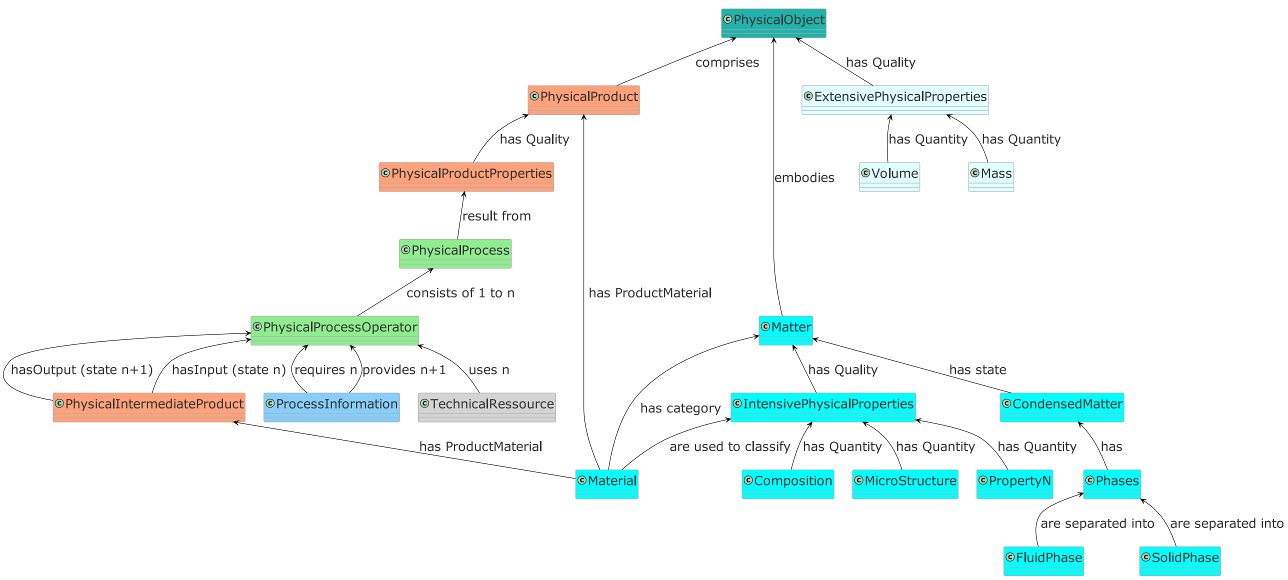


FIGURE 21 | Modeling pattern combining material and process modeling according to VDI/VDE 3682. Green color indicates process/process operator, gray color indicates technical resource, blue color indicates information, red color indicates product, and cyan and light cyan indicate condensed matter related classes.

TABLE 3 | Exemplary competency questions.

What are the as-is values for product x at process step y?
What are the results of an material extrusion process simulation?
Which process steps does process x consist of and which machines are used?
Which material is used in process x and what is the material property value for property y?
Which standards are relevant regarding the characterization of material x?
Which material characterization methods are used for product x
What is the fiber orientation of material x?
Which process steps and machines are necessary for producing product x?
What are the as-is values and their details for product x produced by machine y?
What is change of material properties for product x in process y?
Which material parameters are required for micro-scale simulation x?
Which simulation processes are used for material classes x to z?
Which manufacturing processes is qualified for a material/ product x

4 | OntOMat Ontology and Implementation

For the development of the ontology, we applied the "Simple Knowledge Engineering Methodology" of [40]. It offers good guidelines for an agile modeling process, where a more industrial development alignment methodology, such as [41], could have been applied as well. For brevity, we recapture the main steps introduced by the authors of [40] and provide more details in the following subsections:

1. Domain and scope of the ontology include competency questions (already defined in the previous section) to narrow the scope
2. Reuse of existing ontologies that include 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 a top-down, bottom-up, or combined approach
4. Define properties of classes including "slots" such as cardinality and domain/range
5. Define instances, which include generic instances that should be available for every user, but also include illustrating examples

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

4.1 | 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 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 22 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.

4.1.1 | Upper Ontology

The Industrial Data Ontology (IDO) [42] shows a good fit to the domain/context described above and has a clear focus on industrial products and the product life cycle it was selected as the upper ontology. The IDO defines generic terms for things that exist in more than one industrial domain and supports the modeling of all life cycle phases of industrial assets and processes. However, it fails to provide a detailed concept for describing materials. IDO is composed in the semantic web language W3C OWL 2 [43] and is a part of the new ISO standard ISO/NP 23726 "Ontology Based Interoperability" (ISO/NP 23726-3). In order to enable the IDO as upper ontology for the OntOMat application ontology, it was enhanced with a concepts for materials and process models. This allowed us to model the relation between processes and materials in product generation as well as to model generic material knowledge following the methodology of condensed matter physics.

The IDO was extended by introducing the concept of nominal material, as well as the VDI/VDE 3682 process structure. Together with the already existing concept of Physical Products, this results in a modeling pattern that, for the first time, systematically links the domains of matter (or material), process, and product while simultaneously representing the emergence of product and material instances as a result of processing. This pattern constitutes the core of the OntOMat application ontology and at the same time forms the basis for structuring and specifying the data to be imported into the knowledge graph. IDO differentiates between actual and prescriptive!

4.1.2 | Products, Materials, and Their Properties

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. It is connected by the

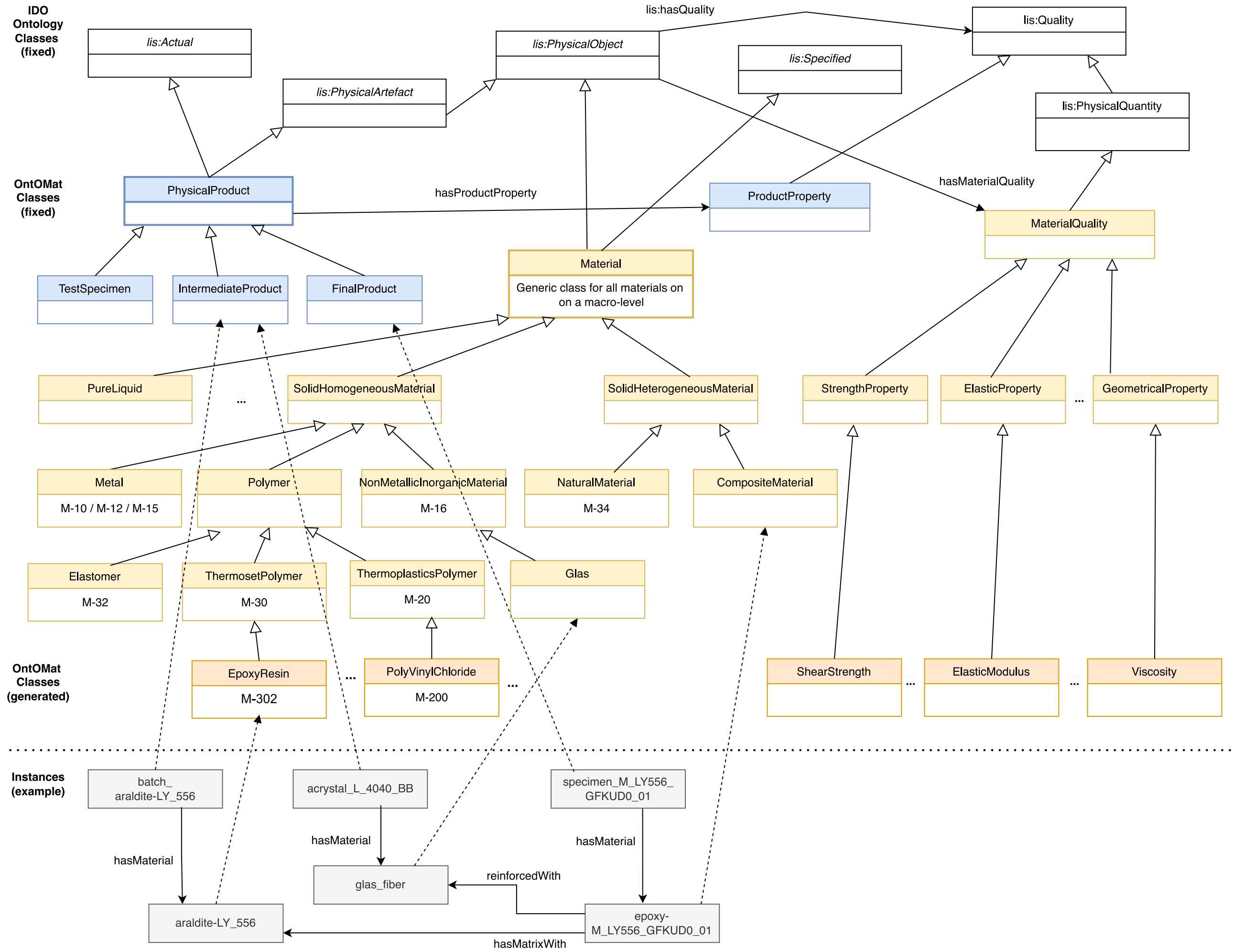


FIGURE 22 | Partial rendering of OntOMat ontology showing the classes for nominal materials, products, and material qualities, where white-headed arrows are sub-class relations, dashed arrows are instantiations of them, and black-headed arrows are objects properties between instances.

`hasMaterial` object property to a physical product. 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. The material class hierarchy 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 IEC standard spreadsheet.[3] The IEC 62474:2018 standard misses some concepts important to fiber-reinforced materials:

- 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.
- No CAS registry number is given, which is used to identify the chemical substances 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 object properties `havingMatrixWith` (a matrix material, e.g., epoxy resin), `reinforcedWith` (a material that is used for reinforcement, e.g., fibers), and `filledWith` (a material that is used as a filler, e.g., air). The above properties are needed to describe possible composite structures that can also be nested.

4.1.3 | VDI/VDE 3682 Formal Process Language

The VDI/VDE 3682 guideline introduces a UML-based data model and a XML-based rendering of the visual language. However, the XML-based rendering is underspecified and does not capture the full complexity of VDI/VDE 3682 process flows, for example, cyclic flows or subprocesses. Similar to [44], we suggest that an ontology-based representation for the VDI/VDE 3682 symbols and workflows, as well as an RDF-based representation of (executed) workflows, are the most promising methods to capture it. Unfortunately, the ontology represented by [44] is not aligned with any top-level ontology. Thus, we anchor our representation of the VDI/VDE 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 23, the class `VDIProcess` includes subclasses such as `ManufacturingProcess` and `SimulationProcess`. Similarly, the class `VDIProcessOperator` includes for instance 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 alterations 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 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 (not giving details on `VDIEnergyStream`):

- 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`
- Technical resource: by `producedBy` with the domain `ProductionAsset`

Several characteristics can be assigned to each process operator and state, for instance, define additional information such a path to a sourec file. The link of state/operator to instances of `VDICharacteristics` class is by `hasCharacteristics`.

Note that our representation does not fully align with the VDI/VDE 3682 language, as some definitions seem redundant. We have not introduced any concept for the system border, since the top level-object `VDIProcess` already represents the system border. The VDI/VDE 3682 language also does not have a next and previous relation for representing explicit process flows. Thus, we introduced these properties for quering explicit process flows. For more details on the ontology and its development, see the SeMatS 2025 paper [45].

4.2 | Implementation

The ontology, in addition to being a glossary for documentation, develops its full impact when combined with knowledge graphs (KGs) that capture large collections of real product, material, and process data. A KG builds the base for integrating all data

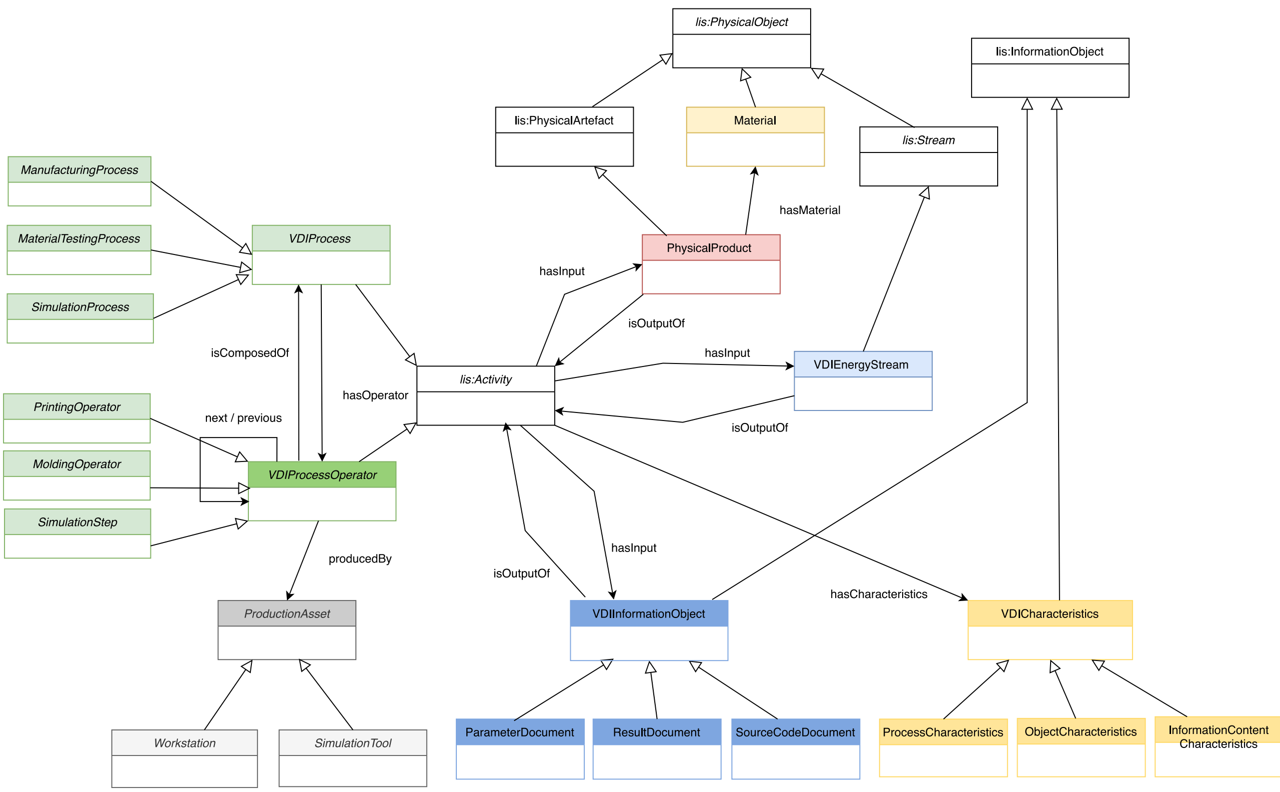


FIGURE 23 | Partial rendering of OntOMat ontology showing implementation of VDI/VDE 3682 formal process description and the alignment with IDO (white boxes), where the arrow coding is similar to Figure 22.

collected along the life cycle of a (material) product. It allows a user to run optimization solutions on top of it, where these solutions could be machine-learning-based, with the advantage of capturing the context of each data item that is encoded in vector embeddings based on the node's neighborhood. First, we illustrate how we implemented the data ingest using the OTTR template language and tooling.[4] Next, we outline the user interaction with the KG, including a web-based user interface (UI) to change the data. Finally, we show a case-study, in which the KG is integrated with simulation workflows to track and evaluate simulation pipelines executed by Abacus FEA.[5]

4.2.1 | *Data Ingest Pipelines*

Data ingestion pipelines, also called ETL pipelines, in OntOMat have two purposes: (a) to create the third tier in the OMO (shown in Figure 22 by orange boxes) based on an Excel spreadsheet for IEC 62474 material classes and a project-specific template for material qualities and (b) to generate RDF-based instance data (also called triples) based on product data and process data. We give more details on (a), but the pipelines for (b) are designed accordingly. As shown in Figure 24a, the original IEC spreadsheet misses unique identifiers, i.e., IRIs, so a preparation step is required to mint IRIs, but also to link the material classes to given parent classes in the OMO (yellow boxes in Figure 22). One pipeline for (a) is illustrated in Figure 24b and consists of the following steps, where the light gray boxes represent the resulting files, the orange boxes represent the steps as Python scripts, and arrows represent an execution of a step:

- Preparation step: implemented as a Python script that outputs a comma-separated values (CSV) text file.
- Class generation step: New classes and their sub-class relations are created based on (prepared) templates of the OTTR language. The templates are run using OTTR tooling[4] with the text files as input.
- Update step: The newly created classes and relations are directly imported into the OntOMat KG.

Note that OTTR templates allow us to generate OWL expressions (such as sub-class relations) but also instance data by using nested templates and an integration with SQL queries over CSV files, which is called batch instantiation of OTTR templates (bOTTR).[6]

4.2.2 | *Data Layer: Standalone KG and API*

For managing and storing RDF triples, any semantic graph database (also called triple store) that supports RDF [46], OWL [43] including (limited) reasoning, and SPARQL [47] can be used. There are many possible choices for a triple store,[7] as we opted for Ontotext GraphDB,[8] respective QLever,[9] when a commercial, respective open-source triple store is required. One requirement for a triple store is the support of OWL 2 reasoning, which is required for the classification of composite materials. Namely, we employ a reasoning regime called OWL 2 RL [43] that allows us to materialize derived classes from the classification described in Section 4.1.

The standard approach for interacting with a KG is by SPARQL queries using the SPARQL-endpoint and the UI of the triple store, which can also be used to insert, delete, and update instances. In the following, we present an example query that returns all material properties, including their quantification for the material called `epoxy _M _LY556 _GFKUD0 _01`:

```
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX ontomat: <https://www.materialdigital.de/ontomat/>
PREFIX ontomins: <https://www.materialdigital.de/ontomat/instance/>
PREFIX lis: <http://rds.posccaesar.org/ontology/lis14/rdl/>

SELECT DISTINCT ?material ?material_property ?material_property_label ? value ?std_dev ?unit
WHERE {
    VALUES (?material) { (ontomins:epoxy_M_LY556_GFKUD0_01) }

    ?material ontomat:hasMaterialQuality ?material_property .
    ?material_property rdf:type ontomat:IntensiveMaterialProperty;
        lis:qualityQuantifiedAs ?quantification .
    ?quantification lis:datumValue ?value;
    OPTIONAL{?material_property rdfs:label ?material_property_label .}
    OPTIONAL{ ?quantification ontomat:standardDeviation ?std_dev .}
    OPTIONAL{ ?quantification lis:datumUOM ?unit .}
}
ORDER BY ?material ?material_property
```

SPARQL can also be used to query the ontology itself. In the following example, we list all possible morphological properties that can be relevant for circular value chains.

```
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
PREFIX ontomat: <https://www.materialdigital.de/ontomat/>

SELECT DISTINCT ?property_class ?label
WHERE {
    ?property_class rdfs:subClassOf* ontomat:MorphologicalProperty ;
        rdfs:label ?label .
}
ORDER BY ?property_class ?label
```

The above queries show that writing complex SPARQL queries is a technical obstacle for the usage and integration of KGs in the material science domain. Hence, we developed a Python-based Flask[10] web application that provides a RESTFul API for external applications and their developers. The API maps HTTP request with parameter to SPARQL queries and also allows to update data in the KG in a controlled manner. For example, the following HTTP POST to .../ontomat/material-properties-by-material with the material ID executes the query shown above and returns a JSON-based result table of all material properties. We believe that the approach of mapping RESTFul API calls to SPARQL queries is a flexible and efficient method to query and update a KG by external applications.

4.2.3 | *Streamlit UI*

The web-based interface intends to showcase the results of the OntOMat project by implementation on a Linux-based infrastructure using Ubuntu Server as the operating system foundation, as shown in Figure 25a. The application stack follows a layered architecture to ensure modularity, reproducibility, and maintainability. At the back-end level, the triple store, as described above, serves as the central data management platform. Above the data layer, an application layer encapsulates the business logic for the user interface, where data access is provided by the RESTFul API introduced earlier. This layer handles ontology queries, data transformation, and validation. The application is deployed as a persistent service using systemd, ensuring automatic startup, fault recovery, and integration into the operating system's service management framework. The presentation layer is implemented using Streamlit,[11] which provides a lightweight web application framework for interactive user interfaces. Streamlit acts as a web server component that exposes HTTP endpoints and dynamically renders front-end components. End users access the system through a standard web browser, which communicates with the Streamlit service as shown in Figure 25b. This layered architecture decouples infrastructure, application logic, and presentation, allowing independent scaling, maintenance, and future replacement of individual components.

4.2.4 | *Question Answering UI*

One feature of the Streamlit-based UI is a chat bot that allows dialog-based interaction with the OntOMat knowledge graph and ontology. The implementation of this feature is, on the one hand, a decision procedure (and fallback) to distinguish between OntOMat related questions and generic questions, and on the other hand, a text-to-SPARQL-query generator (T2SGen) that compiles a given user request/question and the history into the context for a request to a large language model (LLM).

The decision procedure is a boolean classification, performed by the LLM, to decide if a question is aligned with the terms (classes and properties) of the OntOMat ontology. In case the alignment is not given or the SPARQL query generation fails, the request/question is directly forwarded to the LLM. T2SGen is based on the architecture of SPARQLGEN [48], a well established one-shot SPARQL query generator, where we have replaced the sampling module by an "active" ontology compilation module that queries possible

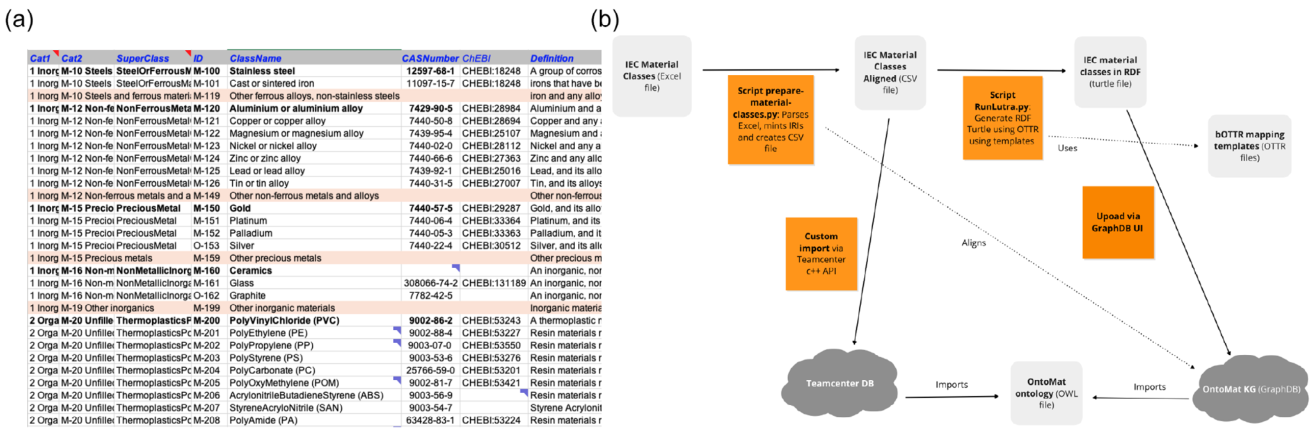


FIGURE 24 | Data ingest for the IEC 62474 material classes and related input Excel data sheet.

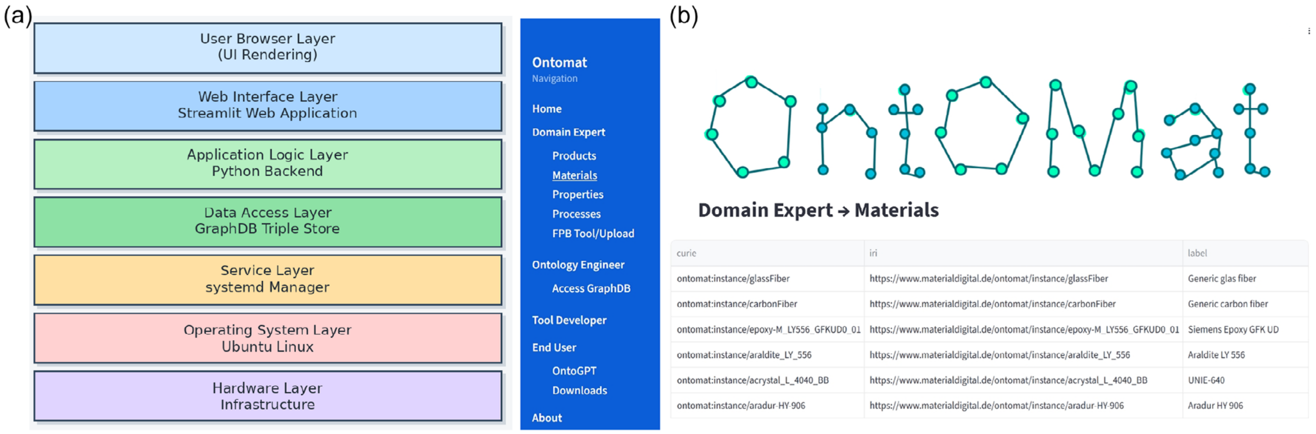


FIGURE 25 | System architecture (a) and screenshot of user interface (b).

classes, object properties, and data properties (using a system query), which are instantiated in the underlying KG, thus only forwarding "active" terms. The compilation includes the filter of too generic terms such as `owl:NamedIndividual`, and will be given in a compressed form to the LLM's context. A generated SPARQL query, if syntactically correct, is then executed using the SPARQL-API of a triple store. The results, depending on the request, are summarized as text or tables and added to the dialog.

For the SPARQL query generation itself, we used OpenAI's gpt-4o and gpt-41-mini,[12] where the language models always create syntactic correct SPARQL, but struggled to capture complex questions that need multiple triple patterns and sub-queries. Note that an approach based on ontology compilation is not as reliable as more recent approaches such as a GraphRAG with RDF2vec [49] or GRASP [50], which also includes reasoning about previous and future steps. the presented approach has the advantage of requiring a very low implementation effort (i.e., about 30 lines of Python code), since at the core there is one system query and an encoding of the results in tabular form. However, for future work, we aim to implement the chatbot as a GraphRAG system and replace T2SGen with GRASP.

Finally, we conducted an initial quantitative evaluation of the query generation time for T2SGen using the OpenAI-interface and the query response time using GraphDB. The experiments were run on a Siemens Azure cloud infrastructure with OpenAI's gpt-4o and gpt-41-mini models installed. The query response time for GraphDB was measured on a Ubuntu 24.04 dual-core server with 4 GB of memory. For measuring the evaluation time, we ran 100 questions of simple (e.g., "Which material classes do you know?") to medium (e.g., "Return all composite materials and their qualities with their datum values and datumUOM.") complexity. The OpenAI-API response for gpt-41-mini ranged between 2 and 5.5 s with an average response time of 4 s. The SPARQL response time was always below 100 ms due to the limited size of the KG and low complexity of the queries.

4.2.5 | Data Layer and UI: PLM System

To demonstrate the practical application of the ontology and data ingest pipeline, Siemens Teamcenter is used as a representative PLM system, leveraging its object-relation data storage and API. As contextual background, this section briefly introduces the underlying PLM infrastructure before describing the extensions made to its data model. Product lifecycle management (PLM) refers to an integrated, information-driven approach to manage all product-related data, processes, and resources throughout the product life cycle, from initial concept and engineering through manufacturing, distribution, maintenance, and end-of-life disposal. At its core, a PLM system is a centralized software platform that unifies all relevant departments, including engineering, production, procurement, quality assurance, and marketing, on a single consistent data foundation. Modern PLM systems are built on a multi-tier architecture comprising a data persistence layer, a business logic layer, an integration layer, and a user-facing presentation layer. Core functional capabilities include structured product data management (PDM), change and configuration management via Engineering Change Requests (ECR) and Engineering Change Orders (ECO), automated workflow and approval processes, full revision history and traceability, as well as standardized interfaces to adjacent enterprise systems such as ERP, CAD/CAM, and MES. Strategically, PLM reduces development cycles through simultaneous engineering, improves project transparency through consolidated real-time product data, and provides the foundation for Digital Twin implementations. To accommodate the requirements of the proposed approach, the native data model of Teamcenter was extended to support the import of material classes, material properties, and VDI/VDE 3682-based process models. Three dedicated importers were implemented for this purpose. The first importer parses an Excel-based IEC 62474 dataset and automatically instantiates all material classes within the PLM system in accordance with the standard. An exemplary result of this import is depicted in Figure A4 in Appendix A, showing a representative material class as created in Teamcenter. Building upon this classification structure, a second importer processes the nominal material templates provided in Excel format, creating the corresponding material objects and populating all defined material attributes as shown in Figure 26. The resulting data structure constitutes a digital twin of each material, enabling consistent and traceable material information management across the PLM environment. To represent VDI/VDE 3682-based process models within the PLM system, a third importer was developed that reads a VDI/VDE 3682-based JSON file, exported from the FPB demo tool, and generates all required objects and their interrelations, preserving the hierarchical and semantic structure prescribed by the standard. Each element of the process description, including technical processes,

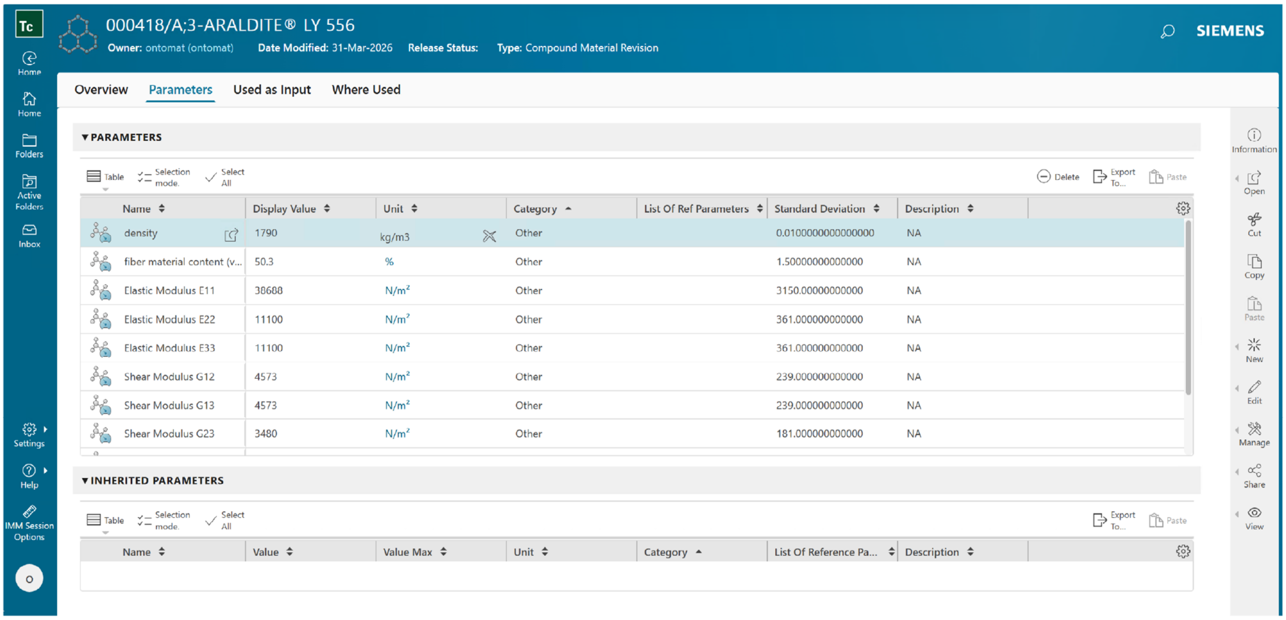


FIGURE 26 | Material object in PLM application after import.

energy and information flows, as well as associated resources, is mapped to a dedicated PLM object type and interconnected through typed relations. This enables the linkage of process, material, and product information throughout the development life cycle, where individual instances can be represented, traced, and managed with fine granularity at each process step. As a result, the imported data faithfully represents the original VDI/VDE 3682 model within the PLM environment, allowing downstream applications such as process analysis, change management, and knowledge retrieval to operate on a standardized and consistent data foundation.

4.2.6 | *KG Integration With Simulation Workflows*

To demonstrate the use of OntOMat in simulation, we implemented a two-step finite-element homogenization workflow in `pyiron`, as illustrated in Figure 27.

With minimal user input (selection of fiber and matrix via IRIs, basic geometric parameters, laminate layup), the workflow queries the KG for constituent properties via a Python-SPARQL API, generates periodic representative volume elements (RVEs), and runs linear elastic simulations in `Abaqus`. First, a micro-structural RVE of a unidirectional fiber composite is analyzed to compute the effective stiffness tensor $\underline{\underline{C}}^{\text{micro}}$. Second, a meso-structural laminate RVE with $n$plies and ply angles ψ_i is constructed using $\underline{\underline{C}}^{\text{micro}}$ to obtain the laminate stiffness $\underline{\underline{C}}^{\text{meso}}$. In both steps, preprocessing, solver execution on an HPC system, and post-processing (extraction of all 21 independent stiffness components) are automated. The resulting effective properties are written back to the OntOMat KG.

The workflow is structured as reusable `pyiron` nodes (initialization, KG query, preprocessing, FEM solve, FEM evaluation,

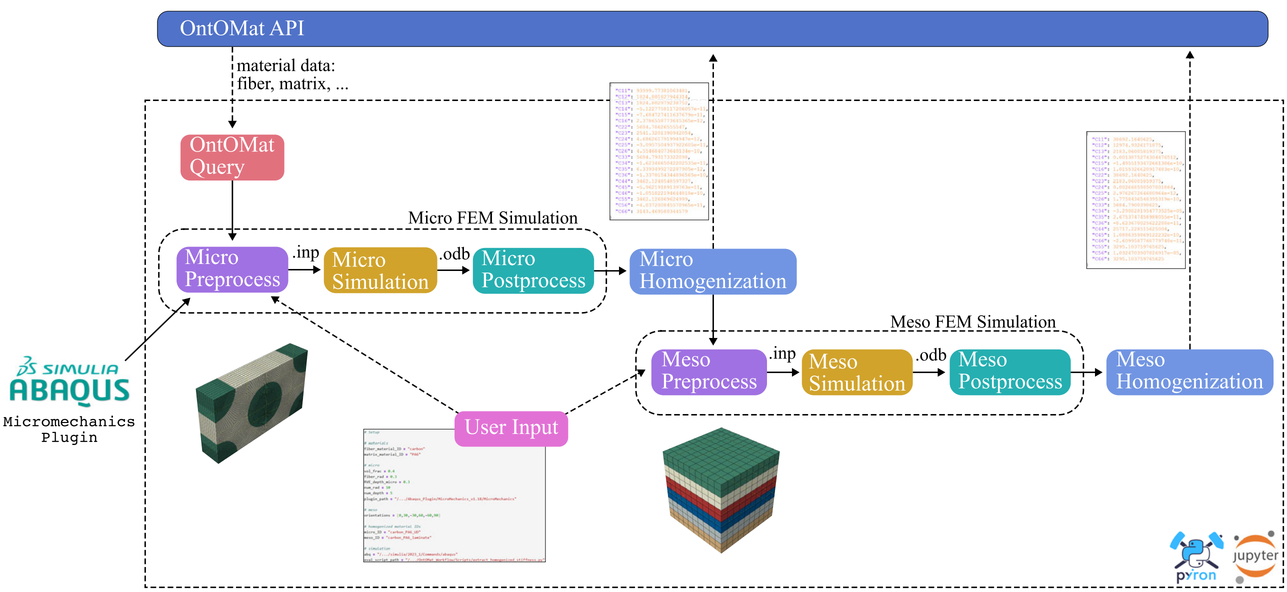


FIGURE 27 | Integration with simulation workflows.

KG upload, finalization) and illustrates how semantic process and material descriptions can drive automated multiscale FE simulations and systematically enrich a materials knowledge graph with simulation-derived properties. The workflow described corresponds to a specific multi-scale simulation process, which was modeled above using the VDI/VDE 3682 tool (cf. Figure 14). Here, the specific workflow was initially generated manually, but future goals include automatically deriving process entities based on their semantic description. This workflow can be used to investigate how a variation in the input parameters (materials or geometry parameters) influences the effective variables at the structural level. It should be noted here that the workflow itself, as described by the VDI/VDE 3682 tool, represents an object of the KG, but nevertheless also makes use of the KG by querying existing data when executing the workflow or writing back newly calculated properties.

5 | Conclusion and Outlook

A domain data model and application ontology modeling the role of materials and material properties in the context of industrial products and their life cycles, as well as the related product design and engineering workflows are presented using the material system of fiber-reinforced polymer matrix composites as an example. It is shown that the dependency of the product material property values from the various processes applied, require the detailed modeling of the relations between the material and process domains as well as the domains themselves. This holds also true for the virtual product model, allowing for direct evaluation of the impact of material property values changes on the related/by the related processes. The established virtual product data model can therefore be regarded as the first step toward the implementation of a model based enterprise (MBE) approach. The process and material model patterns of the developed ontology are generic enough to be applied beyond the chosen material system to describe a wide variety of industrial products, their design engineering workflows, as well as manufacturing, operation and end of life processes. Especially, converting and embedding the VDI/VDE 3682 formalized process description (FPB) into a semantic representation and embedding it into the ontological description allows to model every involved process, including the virtual processes and provides the means to incorporate all life-cycle assessment (LCA) relevant inputs and outputs. Limitations of the VDI/VDE 3682 process description were encountered when modeling virtual, e.g., finite element simulation processes as well as stochastic processes. For those more software-oriented processes, the composition/decomposition capabilities of the FPB are stretched beyond the limits, as iterations and modularity become difficult to model, and the distinction between product and information object is blurred. Following the idea of the virtual product model being the representation (digital twin) of a physical object, we were nevertheless able to model the virtual design engineering processes in a multiscale schema. It was demonstrated that the developed ontology and knowledge graph can be interfaced with a standard LLM (large language model), providing an easy to use query interface avoiding any user defined SPARQL queries. The integrability of the knowledge graph into the industrial PLM application landscape was demonstrated by the expansion of the Siemens Teamcenter IMM data model according to the defined domain data model. This allows the user to add and edit nominal materials as well as VDI/VDE 3682 conforming processes which are stored in the Teamcenter relational database. The data model keeps track of the relations between material and process instances such that the data can be exported into a knowledge graph representation at any time.

5.1 | Outlook

As this paper focused on the development and implementation of the application ontology and the required data ingest pipelines, the evaluation of the knowledge graph performance with regards to the defined competency questions will be presented in future work. Content-wise, this will include the modeling of the recycling process described within this paper as well as the in-situ characterization during the manufacturing process. In this context, one next step will be the enhancement of the VDI/VDE 3682 modeling tool to automate and simplify the modeling of process instances of manufacturing and design engineering processes and direct knowledge graph ingestion. Regarding the interaction with the knowledge graph, besides the existing API, we plan to expose the graph via MCP (model context protocol) either by using the existing MCP implementation of the triple store (e.g., in GraphDB 11.2) or by providing our own implementation based on the Text-to-SPARQL conversion presented earlier. The API will also be leveraged to generate stochastic simulation runs according to the presented stochastic process model and to store the results directly in the knowledge graph for further analysis. Future work on the LLM-based user interface will focus on the visualization of query results in process flow illustration. The current version of the ontology will still be slightly extended to introduce more fine-grained classes, e.g., for production assets or process operators. We deliberately choose to align the OntOMat ontology with the IDO upper ontology, since IDO is wider adopted by particular industries such as oil and gas.[13] Furthermore, IDO employs the same modeling patterns as BFO but also introduces patterns for (a) the product lifecycle of materials including activity, spatial and assembly based break-down, and (b) complex activities that could arise from VDI/VDE 3682-based manufacturing/simulation processes. However, we are also working on aligning the OntOMat ontology with the more material-science-focused PMDCo 3.0 ontology,[14] which should lead to two additional PMDCo application ontologies.

Author Contributions

Nicolas Christ: conceptualization, data curation, investigation, methodology, software; validation, visualization, writing – original draft, writing – review and editing. **Jörg Hohe**: conceptualization, data curation, funding acquisition, investigation, methodology, resources, validation, visualization, writing – original draft, writing – review and editing. **Martin Kördel**: conceptualization, data curation, funding acquisition, investigation, methodology, project administration, resources, supervision, validation, visualization, writing – original draft; writing – review and editing. **Michael Giese**: conceptualization, data curation, investigation, methodology, validation, visualization, writing – original draft, writing – review and editing. **Niklas Toffert**: conceptualization, data curation, investigation, methodology, software, validation, visualization, writing – original draft, writing – review and editing. **Christian Seidel**:

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Acknowledgments

OntOMat (funding code 13XP5197A) and PMD-X MAPRO (funding code 13XPM506C) are funded projects of the Federal Ministry of Research, Technology and Space (BMFTR) as part of the German Platform Material Digital (PMD). The TLGI was funded by the Federal Ministry for Economic Affairs and Climate Action (BMWK) for the "Promotion of Innovation Competence with Non-Profit Industrial Research Institutions" - INNO- KOM Module "Investment Grant for Scientific and Technical Infrastructure" with the funding code 49IZ190032. Similarly, the X-ray cabin with integrated development platform has been funded by the BMWK in the framework of the INNO- KOM Module "Investment Grant for Scientific and Technical Infrastructur" with the funding code 49IZ240042.

Open Access funding enabled and organized by Projekt DEAL.

Funding

This work was supported by the Bundesministerium für Forschung, Technologie und Raumfahrt (13XP5197A) and the Bundesministerium für Wirtschaft und Klimaschutz (49IZ190032, 49IZ240042).

Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

The data generated in this study will be published openly on https://dataportal.material-digital.de/ and https://github.com/materialdigital/ontomat-data_collection.

Endnotes

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Appendix A

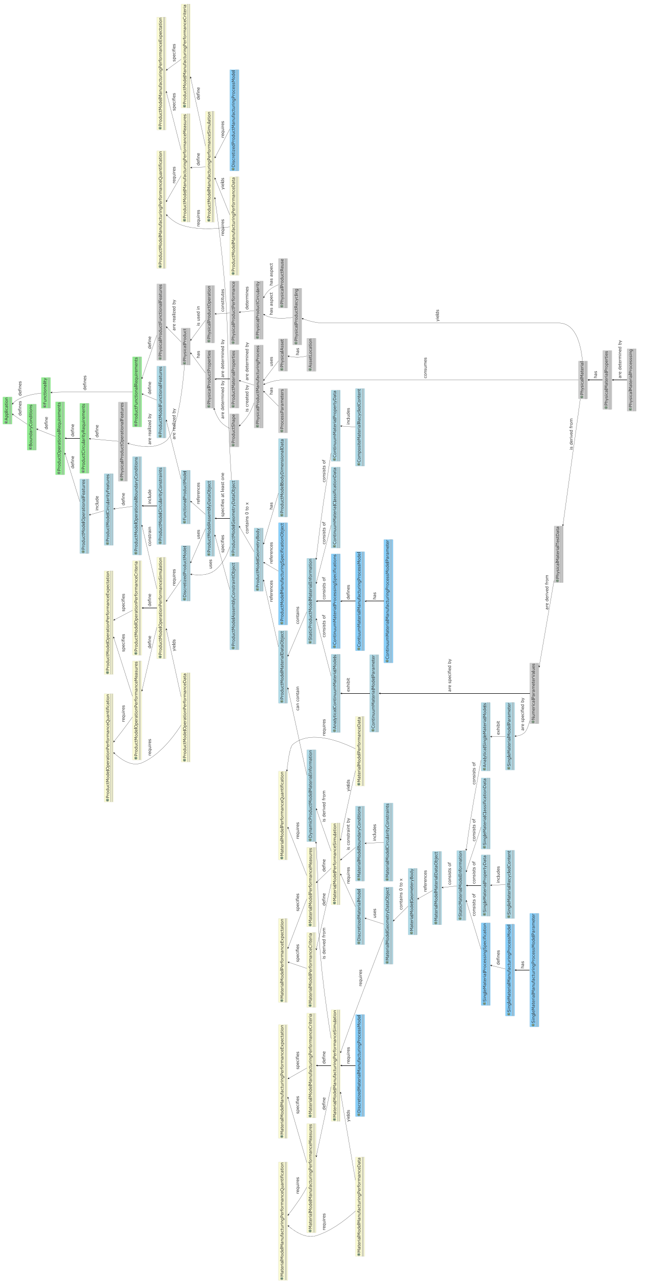

FIGURE A1 | Combined domain data model. Color coding according to Figure 9.

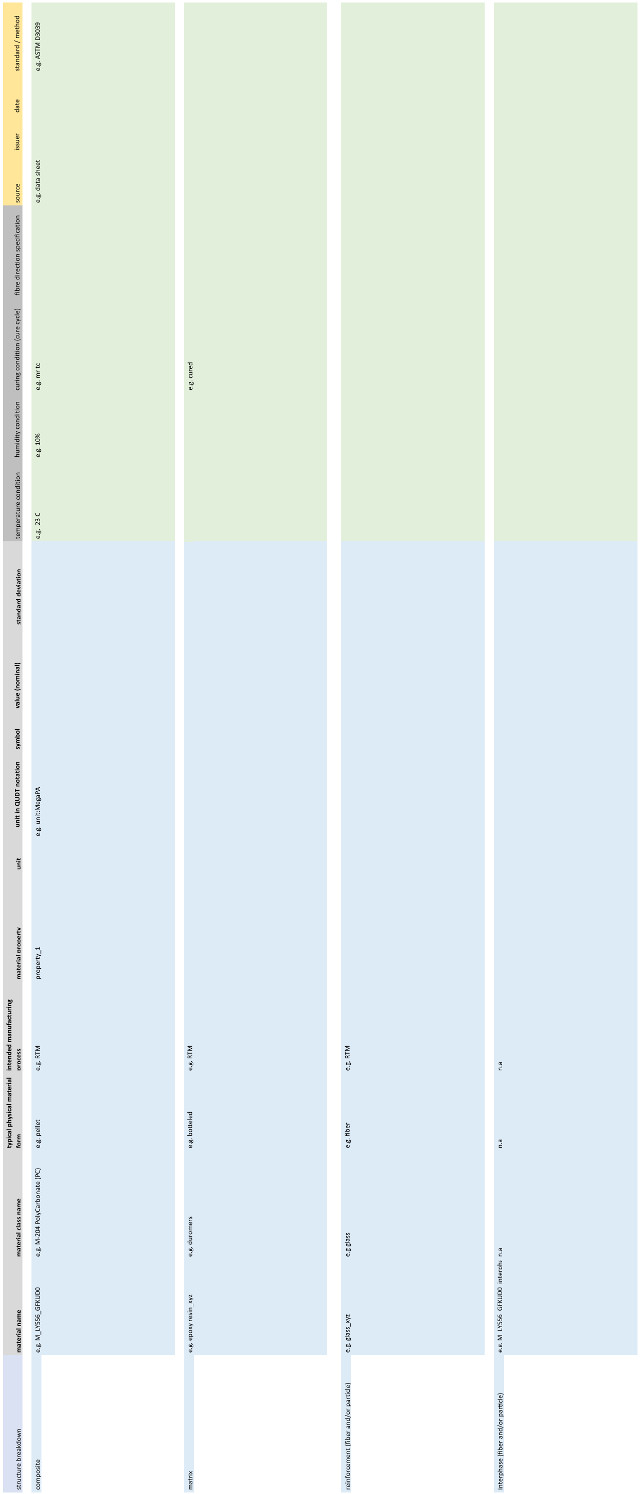

FIGURE A2 | Partial view of nominal material template.

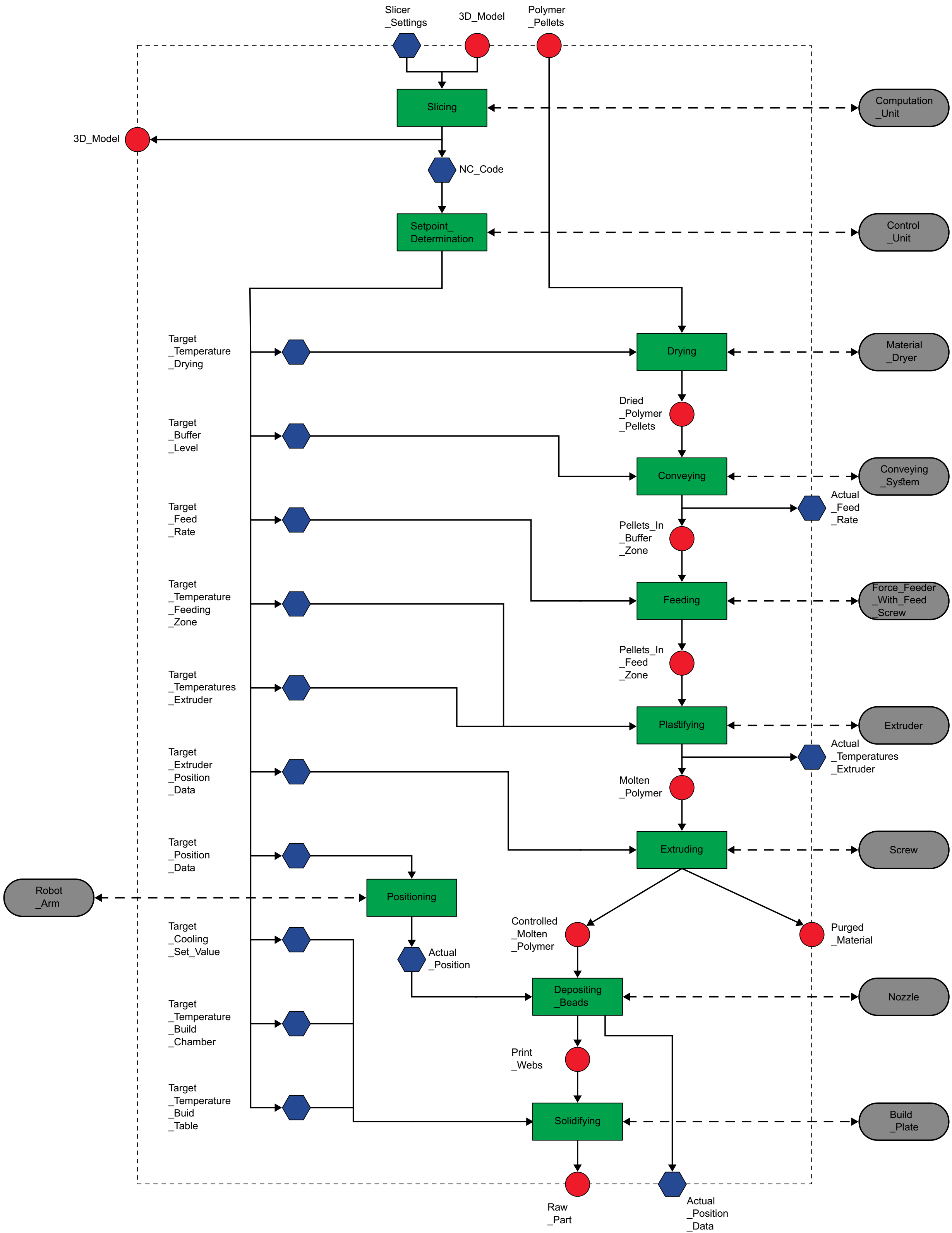

FIGURE A3 | Formalized process description of the (simplified) MEX process.

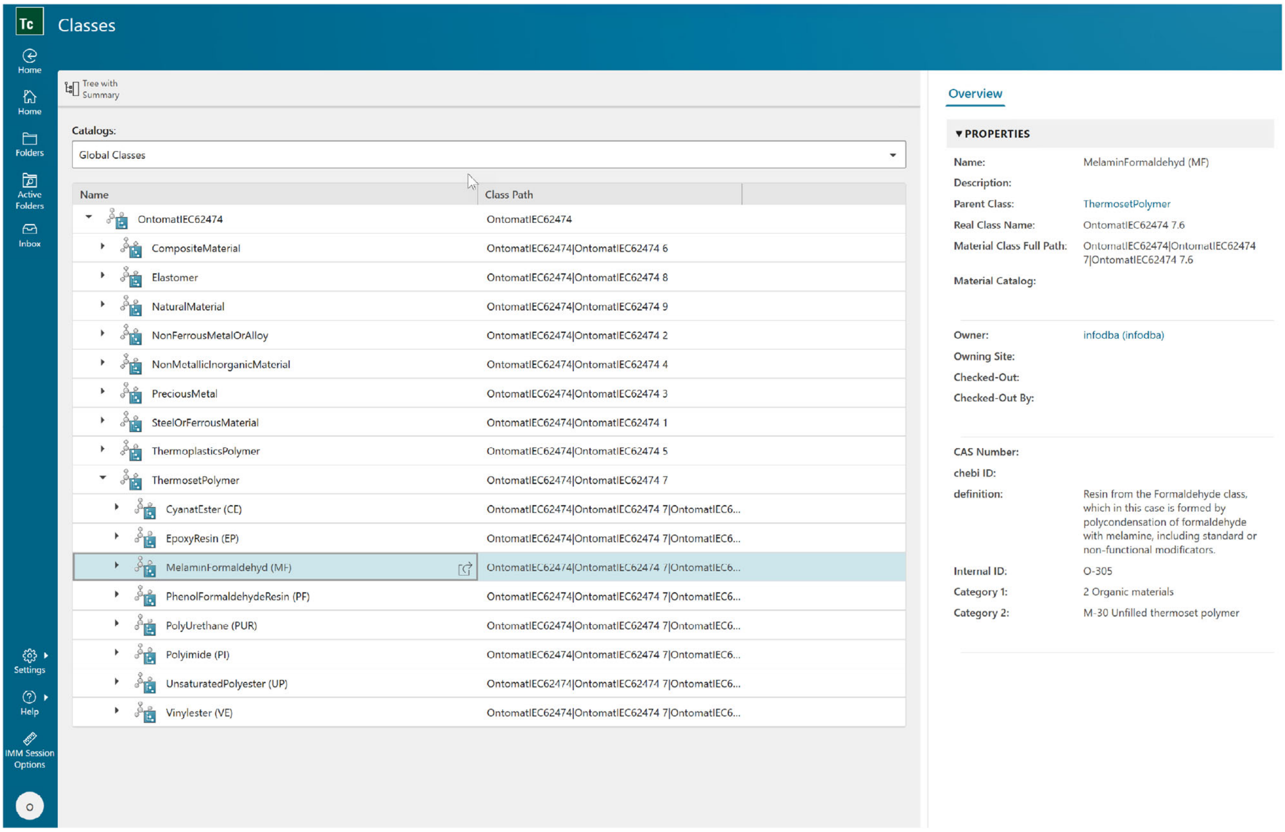

FIGURE A4 | IEC 62474 Material classes in PLM application.