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Toward a Li-Ion Battery Ontology Covering Production and Material Structure

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An ontology for the structured storage, retrieval, and analysis of data on lithium-ion battery materials and electrode-to-cell production is presented. It provides a logical structure that is mapped onto a digital architecture and used to visualize, correlate, and make predictions in battery production, research, and development. Materials and processes are specified using a predetermined terminology; a chain of unit processes (steps) connects raw materials and products (items) of battery cell production. The ontology enables the attachment of analytical methods (characterization methods) to items. Workshops and interviews with experts in battery materials and production processes are conducted to ensure that the structure is conformable both for industrial-scale and laboratory-scale data generation and implementation. Raw materials and intermediate products are identified and defined for all steps to the final battery cell. Steps and items are defined based on current standard materials and process chains using terms that are in common use. Alternative structures and the connection of the ontology to other existing ontologies are discussed. The contribution provides a pragmatic, accessible way to unify the storage of materials-oriented lithium-ion battery production data. It aids the linkage of such data with domain knowledge and the automation of data analysis in production and research.

1. Introduction

Electrochemical energy storage combined with renewable energy sources is the sustainable solution to the current energy crisis and mitigation of the geopolitical and environmental consequences resulting from the current dependence on fossil fuels.[1] Early material and technological advances in battery research[2,3] combined with their portability have made batteries the frontrunner in energy storage; from an enabling technology for mobile computing and consumer electronics to the backbone of electric vehicles, large-scale intermittent energy storage, and smart grids. The availability of structured battery data plays a vital role in battery production, development, and application. It can contribute to investigating new electrode materials, optimizing cell design, improving the battery manufacturing process, modifying

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battery testing conditions, reducing costs, improving cell quality, and expanding battery application fields.[4,5] Today, battery development is based on dedicated research, informed decisions, and trial-and-error.[6] Given the accelerated pace of innovation and huge financial investments in battery research around the world, this approach is ineffective in bringing about the transformative changes that are urgently needed. With the targeted mining of the vast amount of data and information in the field of battery cell production and battery materials, this issue can be aptly addressed and overcome by digitalization and modern informatics. Artificial intelligence (AI), exemplified by machine learning, could accelerate this process by analyzing the data and making predictions.[7,8] However, further processing and application of battery data by artificial intelligence are still hindered by the lack of a common vocabulary and interoperability.[9] Although the problem is already well defined, there is currently no complete solution.[10] Formulating a material and production ontology is a prerequisite for building a comprehensive battery database infrastructure.

An ontology can be defined as a formal, explicit specification of a shared conceptualization,[11] a machine-readable abstraction of a domain, built on consensus between different people, revealing constraints, relationships, and dependencies of and between the concepts. The primitive elements of one ontology include concepts, attributes, relations, constraints, instances, and axioms.[11] An ontology can support achieving data interoperability by defining a common vocabulary, which can serve as a basis for a machine-readable knowledge graph.[12] While an ontology can additionally contain a hierarchical structure of *is-a* relationships between concepts, an ontology also contains other, often richer, kinds of relationships.[11] Hierarchical structures are often referred to as taxonomies. Taxonomies and ontologies can help to organize and structure knowledge in the research area and the battery industry. Also, the rapid development and building of Gigafactories require efficient data management for efficient monitoring that can be aided by structuring data generated during production with common ontologies.

The elementary multiperspective material ontology (EMMO)[13] is a multidisciplinary top-level ontology for applied sciences. The main subject in EMMO is matter (atom, molecule, material, continuum, etc.) and its properties. The physical properties are linked to the matter via the semiosis process when the interpreter observes the result of the measurement and assigns a meaning (sign) to the corresponding material property. EMMO, as a top-level ontology, has been utilized in two battery domain ontologies: battery interface ontology (BattINFO)[14] and battery value chain ontology (BVCO).[15] BattINFO, developed in the Battery Interface Genome—Materials Acceleration Platform (BIG-MAP) consortium,[16] extends EMMO by adding electrochemistry field knowledge. It introduces concepts such as an electrode, electrochemical interface, half-cell/full cell, electrochemical processes, and reactions described by corresponding physical laws and battery measuring techniques. The BVCO is being developed in Fraunhofer Institut für Silicatforschung (ISC) and implements knowledge in the battery production area, from raw material mining to battery manufacturing and battery recycling. The battery value chain consists of production steps and elements such as raw materials and components, which serve as inputs for production steps, and as outputs for others. The German research cluster ProZell developed a battery life cycle-oriented ontology containing one battery taxonomy and one LifeCycleStage taxonomy.[17]

Here, we focus on the structuring of data on materials and intermediate products that occur in the production of batteries in the laboratory and factories. Current ontologies in the battery domain are relatively abstract and/or focus on chemical and physical processes that do not produce data in production. They require additional definitions to link to the type of data currently available. This contribution presents a pragmatic approach to the description of the battery production process that connects a material-oriented and a process-oriented view. We used an interactive process with interviews and workshops to identify consensus terminology for generalized processes (steps) and starting/intermediate products (items) in lithium-ion battery production. The ontology engineering as described in ref. [18] was loosely followed to structure the process. After identifying problems and opportunities for data modeling (the feasibility study part of the ontology engineering meta-process), workshops and conducted interviews were carried out to develop competency questions,[19] consensus on a glossary, and reference processes (the Kickoff part of the ontology engineering meta-process) to create a semi-formal ontology.

The ontology was created as a middle-out approach, where the concepts from relevant data items and processes of the consortium were collected and used to build the ontology. The term “material” is not consistently used in the domain, and we developed a description that avoids the term but can immediately be connected to materials analyses as they are used in battery production. The resulting ontology introduced here is generic enough to cover battery production at an industrial scale and the small-scale manual fabrication typical for research work. We discuss how the ontology can describe the nature of analyzed samples and manage the resulting data in a connected form covering the battery production process and applied analytical methods. It has been designed to be converted into more formal descriptions where necessary and to be mapped to the terms used in higher-level ontologies such as BattINFO, EMMO, and BVCO.

2. Results and Discussion

2.1. Process Ontology: Steps

The interviews on the glossary and the reference process indicated a considerable heterogeneity of manufacturing approaches. The processes vary depending on the scale of battery production.[20] It was possible to identify broadly accepted terms for process steps. They summarize different specific implementations of processes that are typical for battery production. Thus, we created a prototype ontology based on a process-oriented view that is compatible with a broad range of production approaches. It was then further refined using an input of collaborators from different fields of (applied) battery research. The prototype ontology was aligned with a reference production process that is used at the “Battery LabFactory Braunschweig” (BLB) and was verbally described and graphically depicted as a series of sequential processes.

The resulting structure had a process-engineering focus. Our goal was to provide an ontology that is equally useful for the description of the materials and intermediate products of battery production. Therefore, we increased the level of abstraction and introduced the term "step" as a generic and uniform description of any process that has defined input and output. This abstracts typical steps from specific machinery that can be very different at small laboratory scale and larger production scale. The modified ontology makes it easier to vary the process chain by including or excluding certain steps in the process, too. This ensures that, for example, a user working on a small scale can effectively skip a production step while still describing their process with the same ontology. Similarly, a pilot plant scale user can omit a certain material characterization while following their production with this ontology. Another important feature of the current ontology is that it is structured as a series of consequent, interconnected process steps that have their discrete locations in the process chain. The ontology thus provides a classification of terms (names of processes and products) and a logical structure that defines the terms. The representation of the production process can be seen as a logical connection of process steps that replaces an unsorted list. The additional level that this ontology provides offers better categorization because a single isolated step in this ontology cannot be self-sufficient as it cannot result in a complete product, in this case, a battery cell. This chain of steps is connected with the items representing raw and intermediate materials.

The ontology covers the subprocess of electrode production (**Figure 1**) which contains six steps.[21] It starts by homogenizing and structuring dry components of an electrode (namely active material and conductive additive(s), optionally binder(s)) in a step of dry mixing. This step influences the pore structure of the electrode by altering the agglomeration grade of conductive carbon black, a commonly used conductive additive in electrodes. Depending on the mixing intensity and the properties of materials, the surface of the active material is coated by a carbon black or a carbon black/binder network.[22,23] The powder mixture resulting from this process step is combined with a solvent in the next step—wet mixing. During wet mixing, the binder gets dissolved, a final deagglomeration of carbon black is taking place, and the viscosity of the electrode suspension (slurry) required for the optimal coating is obtained.[24,25] The slurry is then coated on

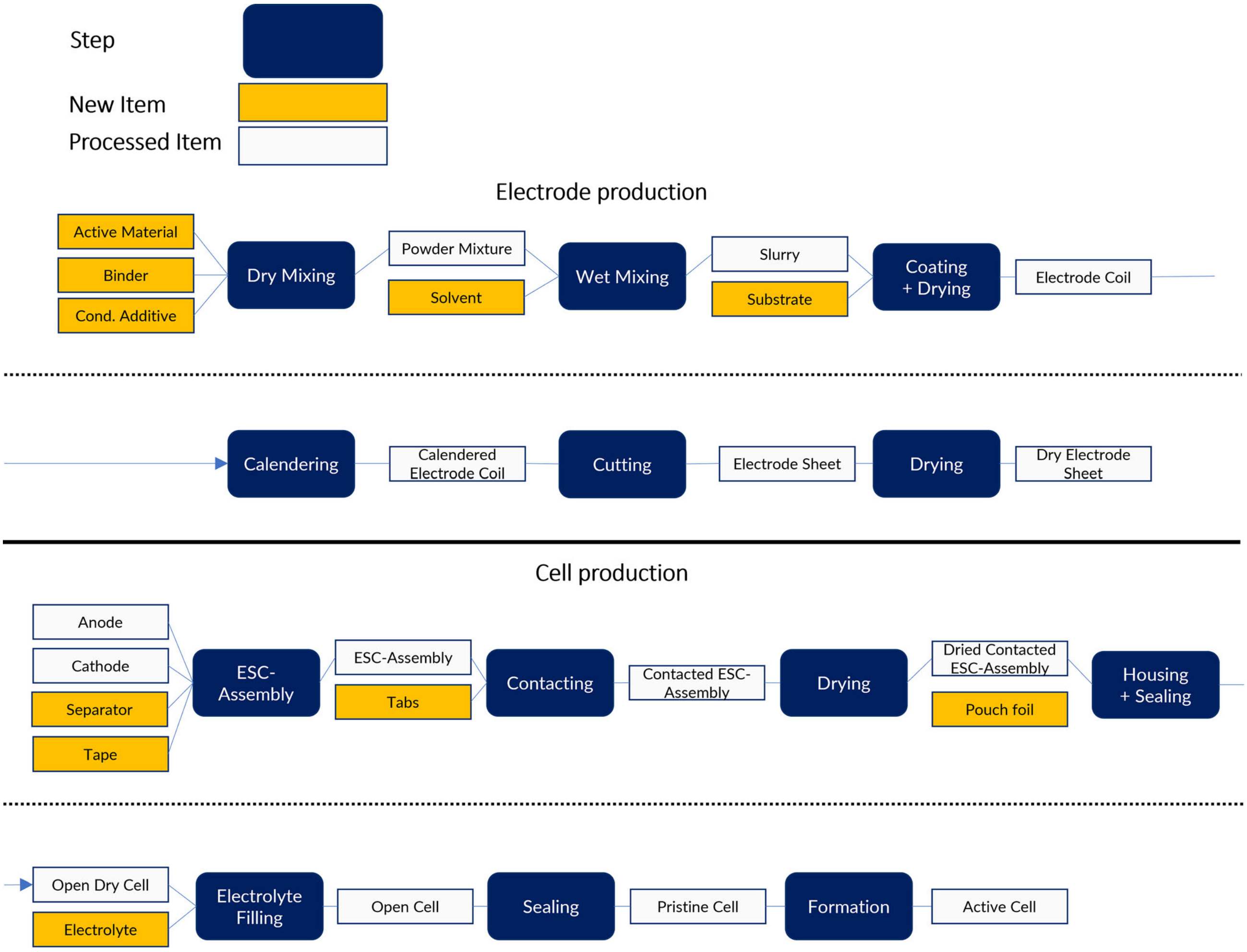

Figure 1. Visual representation of the full ontology covering the subprocesses electrode production and cell production.

the substrate (an aluminum foil for the cathode and a copper foil for the anode) in the coating step, where homogeneous coating and good adhesion to the substrate are crucial quality features.[26,27] The coating on the substrate is subsequently dried in the drying step which needs to ensure efficient and complete removal of the solvent without deteriorating the homogeneity of the coating, especially without a segregation (or migration) of binder and conductive addtitive to the coating surface.[28,29] Coating and drying are merged into one step in the present ontology, because usually continuous coating lines with integrated drying units are used, as is the case in the reference process. The resulting electrode is rolled onto a coil, resulting in an electrode coil. The electrode is usually compacted in the next step, calendering. Calendering establishes the final microstructure, density, and mechanical homogenization of the coating, and adjusts the future ionic and conductive transport pathways of the electrode.[30,31] The resulting calendered electrode coil is cut to suitable dimensions in a cutting step that should preferably have no influence on the quality of the electrode.[32] Before the cell assembly process, electrode sheets are dried again to remove the remaining moisture and other adsorbed species from the atmosphere that could negatively affect the electrochemical performance of a battery. Note that in industrial processes, the final drying is often carried out before cutting by drying entire electrode coils.

The subprocess of cell production begins with the assembly of the electrode–separator–composite assembly (ESC Assembly), followed by contacting, drying, housing and sealing, electrolyte filling, sealing, and finishes with formation.[21] In the first step (ESC Assembly), the dry electrode sheets are joined together with the incoming separator to form an ESC Assembly, which is fixed using a tape. Several process variants such as stacking, *z*-folding, or winding can be considered for this step. Depending on the choice of process variant, the resulting ESC Assembly may be either cylindrical (round winding) or prismatic (stacked, *z*-folded and flat winding).[33] The current collector flags of this ESC Assembly are then connected to external tabs in the next step (contacting) and form the poles of the battery cell. The resulting contacted ESC Assembly is then dried in a vacuum oven. It is worth mentioning that in industrial processes with short residence times of the ESC Assemblies in the dry room, no additional Drying step takes place. Residual moisture would react with the electrolytes' conductive salts (LiPF6) generating hydrofluoric acid (HF), which in return would degrade the battery cell.[34] In the reference process, the dried contacted ESC-Assembly is then placed in a housing consisting of Pouch foil which is prepared by thermoforming and impulse sealing (housing and sealing). The resulting assembly remains open on one side for the subsequent step of electrolyte filling and is referred to in the following as an open dry cell. In the next step, the electrolyte filling, the open dry cell is filled with electrolyte and finally sealed using impulse sealing.[35] The final step of formation completes the cell production process chain by activating the inactive pristine cell and results in the active cell as the final item. Depending on the cell type and chemistry, the cells might remain opened during formation, after which the formed gas is removed from the cell, and further electrolyte is filled into the cell.

2.2. Component Ontology: Items

The abstract step unifies different versions of processes and makes it easy to combine processes that are seen as a unit, e.g., because they are performed in the same machine. A similar abstraction is useful to unify the materials used in electrode and cell production and intermediate products that are produced and modified in steps. We introduce the object-oriented term "item" to represent these objects. We avoid more specific terms such as "raw material" or "product" to avoid confusion: items can be the product of one process and raw materials for the next process in existing nomenclature. Almost all objects in the electrode and cell production process, including objects often referred to as raw materials, such as active material powder, have already been processed and modified before they are used in the production process.

We prepared a list of items that summarize raw materials and processed products (see **Table 1** and **2**). Each item is defined only by its name. It proves difficult to find unique names that would unequivocally define individual items. Our interviews showed that commonly used item names can remain the same even if the processed item is modified by several processing steps, like, electrode sheet before and after calendering. To date, there are not any published standard of terms for battery objects that have been agreed upon in the battery research community. Names for the items provided in Table 2 have been assigned after evaluating

Table 1. List of process steps included in the current ontology.

Process step name	Description of the step
Dry mixing	Homogenization and structuring of dry components of an electrode.
Wet mixing	Combining the powder mixture with a solvent, creating a slurry.
Coating and drying	Coating of the slurry onto the substrate (current collector), including subsequent drying.
Calendering	Compaction of an electrode to a final density.
Cutting	Cutting an electrode coil to target dimensions (electrode sheet).
Drying	Removing the remaining moisture in the electrode sheets before further cell assembly
ESC Assembly	Joining the components into an electrode–separator–composite (ESC) assembly
Contacting	Welding the current collector flags to the external tabs to form the battery poles
Drying	Extracting any remaining moisture in the ESC Assembly before filling
Housing and sealing	Forming the pouch housing by deep drawing and impulse sealing as well as inserting the dried contacted ESC Assembly
	The dried contacted ESC Assembly
Electrolyte filling	Injection of electrolyte into the open dry cell
Sealing	Final closure of the open cell by impulse sealing
Formation	Formation of the (inactive) pristine cell to form the solid–electrolyte interface (SEI)

Table 2. List of items used in the suggested ontology.

Item name	Description of item
Active material	Powder that stores lithium ions in the electrode and performs the electrode reaction
Binder	Binding agent added to achieve adhesion in the electrode
Conductive additive	Additive that ensures the electrical conductivity in the electrode
Powder mixture	Mixture of dry components needed for slurry production
Solvent	Solvent used for dispersing the powder mixture and dissolving the binder
Slurry	Electrode suspension for application on the substrate
Substrate	Current collector; an electrically conductive foil on which the slurry is coated
Electrode coil	Dried slurry—substrate compound before calendering
Calendered electrode coil	Electrode coil compacted to the target density
Electrode sheet	Electrode sheet cut to the target geometry
Dry electrode sheet	Electrode sheet after drying
Cathode	Dry electrode sheet for the positive electrode
Anode	Dry electrode sheet for the negative electrode
Separator	Ion-permeable membrane between cathode and anode, preventing electrical contact
Tape	Temporary adhesive strip used to fix ESC Assembly
ESC Assembly	Compound of anodes, separators, and cathodes
Tabs	Metal strips, which allow electrical contacting of the cell
Contacted ESC Assembly	ESC Assembly contacted with tabs
Dried Contacted ESC Assembly	Contacted ESC Assembly after drying step
Pouch foil	Material (foil) used to enclose the dried contacted ESC Assembly
Open dry cell	ESC Assembly contacted with tabs inside pouch foil casing—before electrolyte filling
Electrolyte	Liquid (conducting salt, solvent, and additives) medium for ionic conductivity
Open cell	Assembled cell filled with electrolyte before final sealing
Pristine cell	Assembled and sealed cells before formation
Active cell	Cell after formation
Aged cell	Cell after it has undergone certain use, test, or targeted aging.

the interviews with the researchers from the various project partners.

Only names are insufficient because process routes and sequences of processes can vary. It is possible to create exact definitions for each item, but the effort would be considerable, and it is highly questionable whether the communities will accept redefined terms. We propose a pragmatic alternative. Items in our ontology are defined by their position within the process ontology and their connection to steps. The position in the process ontology defines the spatial and temporal relationships of the item. All steps and items are related to each other in this way. This makes it possible to uniquely assign all items to each other, to trace individuals along the entire manufacturing process, and to find process–structure–property relationships. The item's position (I) and name (II) define it. A number of properties (III) describing the item are connected to it in the ontology. Properties include data on characteristics of the item that are provided by data sheets and the results of analyses performed during the process, for example. An extendable list of properties has been developed and is provided for each item in the database.

The resulting ontology is more suitable for digital data storage than other ontologies, but the implicit definition of items comes at a cost. It requires reliable links between nonunique item names and correct attribution of properties (often identical) to different items. It is best used with the support of a digital graphical interface that guarantees connectivity and automatically warns of inconsistencies and a database that enforces the linkage of property data to valid items.

2.3. Battery Production Ontology

In the following, we provide a full description of the ontology covering lithium-ion battery production and material data that was constructed using the methods and reasoning explained earlier. The ontology consists of two main entities that have been introduced in Section 2.1 and 2.2 and that are directly connected within the production process. Additionally, the entity characterization methods, connecting information about applied analytical methods on items, are introduced. Each entity contains several defined properties that are also explained in the following sections.

2.3.1. Entity Items

Items are directly connected to at least one process step and can be input, output, or both of a specific step. Items can be connected to two process steps, usually as an output item of one and an input item of the following process step (intermediate product). Each item is associated with properties determined either by experimental methods or from data sheets provided by the material manufacturer or supplier. In the current state of ontology, items are only classified in a first hierarchical level, allowing more flexibility in usage. Extending the ontology by introducing a detailed taxonomy of items is planned.

2.3.2. Entity Steps

A step refers to a specific phase of the battery production process. Several steps can be combinded into a single step or split into multiple steps, depending on the degree of abstraction. The proposed ontology uses a reference process that combines the most common steps in the battery production process at the BLB with common practice in small-scale battery production. A step uses one or more input items to create one or more output items. In the proposed ontology, a step always yields one output item. It may be extended, e.g., to include waste and production scrap.

Each process step has several properties, which can be input properties for setting the machine or output properties generated by a device. A step is not necessarily linked to specific machinery, as it can be a manual step performed by an operator.

2.3.3. Entity Characterization Methods

A characterization method is an additional entity covered in the presented ontology. Characterization methods are defined as performed analytical methods according to the item and are therefore connected to the entity items. Similar to steps and items, properties are attached to the specific methods. Performed analytical methods can be seen as a process of extracting information while following a specific procedure. In ontology, the processes within a characterization are not further defined. Characterization methods can be applied to each item in the ontology.

2.3.4. Entity Properties

Information is stored in properties (data fields) that are linked to items, steps, or characterization methods. Items may be linked to specifications of the manufacturer, time stamps, and identification codes (IDs). Steps may be linked to specifications of the production machine, input settings, output generated by the machine, timestamps, and IDs.

A characterization method that is linked to an item documents the input and output properties of the analysis performed, such as analytic settings and results. A typical minimal implementation will provide a time stamp, a textual description of the method, and a link to a file. An advanced implementation document will describe the entire analytical workflow through a detailed ontology of the measurement technique.

A relation is made from the item to the characterization method. Through this relation, a correlation is established between the entity's steps, items, and characterization methods. All information in the ontology is connected as a knowledge graph. Data produced with this method is then linked to the item via the method description. The ontology contains more than 500 properties attached to items, steps, and characterization methods.

The combination of these entities results in the full ontology covering the structural information in a battery production process. In **Figure 2**, a high-level explanation of the entities and their relations is depicted. Data can be included by inserting the information in the already defined properties, which can be seen as a process–item–characterization method–property relation structure allowing at the same time flexibility and restrictions to enable the comparability of data. The properties connected to an individual step, item, or characterization method are defined. Figure 1 shows the high-level representation of the ontology with the reference process as a basis. The process was split into the subprocesses "electrode production" and "cell production". According to the presented structure, data can be attached as properties to each process step and item. An example can be seen in **Figure 3**.

3. Conclusion and Outlook

We introduce an ontology that describes the production of lithium-ion batteries and supports the management of data on materials and process steps. It is flexible enough to structure data both from industrial or industry-oriented production and laboratory-scale research on batteries. A sequence of structured interviews, workshops, and reviews was used to create a consensual glossary and identify a minimum overall structure for the description.

We introduce generalized steps and items to abstract the battery production process and the materials and assemblies involved. This level of abstraction is pragmatic and accessible, but the term "item" avoids uncertainties connected to the use of terms such as material, product, or assembly that have different connoted meanings in different communities. "Steps" are close to well-accepted process steps of process engineering but avoid the implications; a manually performed step can replace a fully automated one and still yield an overall process structure that is easy to compare. Both steps and items are easily linked to the existing ontologies and lists that describe, for example, analytical methods, processing details, and commercial products. Process instances can be created based on the proposed ontology and according to data structure.

The overall ontology was discussed with experts in the field during multiple workshops to ensure compatibility and usability. It goes beyond existing ontologies and introduces logical links between process steps and materials, but this logic is still basic. Current research investigates which relations are (according to domain knowledge) important enough to be directly codified and in which cases automatic reasoning or consistency checking is realistic and useful. For example, basic physical concepts such as mass and energy balances can be represented using suitable relations between steps and items. This provides links to the

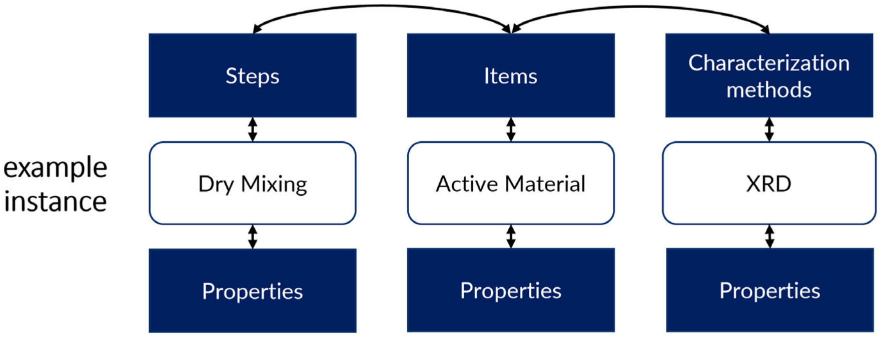

Figure 2. Graphical representation of the entities and their relations in the presented ontology.

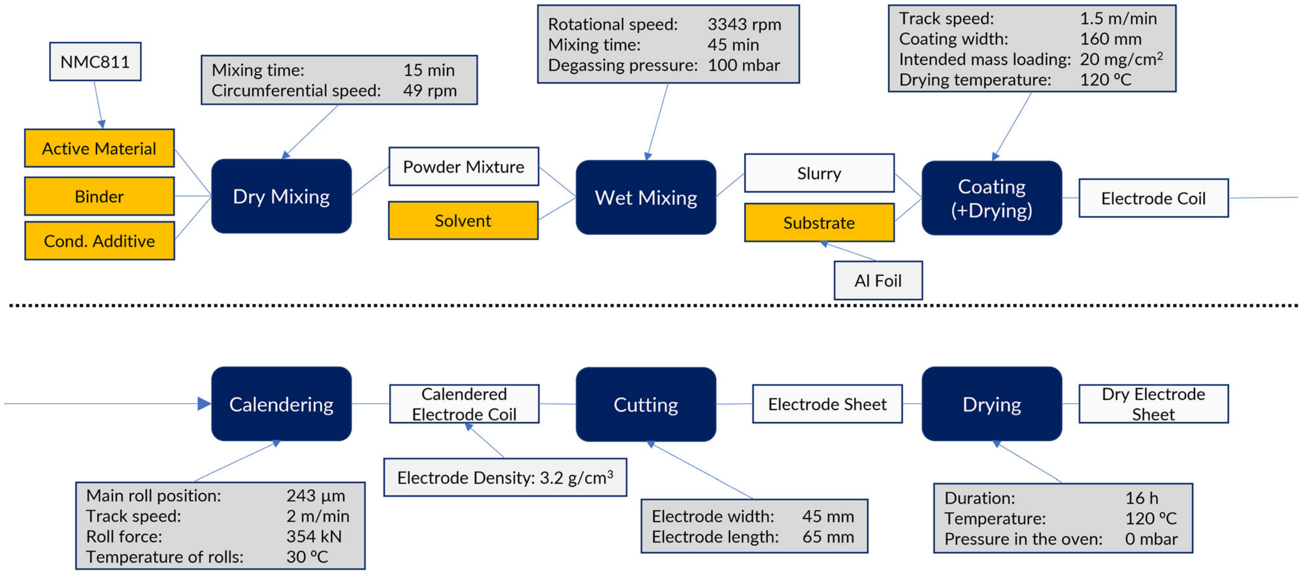

Figure 3. Visual representation of the subprocess electrode production on the specific example of cathode production including corresponding properties.

existing models that describe, e.g., the energy consumption of battery production, cost models, or process control systems that aid engineers running the cell production machinery.

A sequence of steps can be used to define the history of items and identify them. This leads to different levels of digital twinning: a simple documentation can only list which steps were used, without any process data; a detailed digital twin contains detailed process data and even machine states. This provides the flexibility that is necessary to use the same structure for research, production, and end-user documentation. A recent report[36] makes a solid case for digital twins as a technical tool in the digitization of battery manufacturing pilot lines. The classification of battery metadata sets a software infrastructure in parallel with the hardware. In this way, the design of experiments with analytical tools can grow the digital twins through data analysis for optimization of new batteries and their production.

The primary application of the ontology introduced here is the management of material and process data that is generated in battery research and production. It can connect the ad hoc process flows that are currently created, often by the users, to manage data and samples. Other use cases include documentation and teaching, standardization, and the identification of gaps in research and development.

In the near future, an extension and application phase for the ontology engineering metamodel is planned as part of the DigiBatMat project. In the field of dynamic battery research, the expansion and application of ontology will be an ongoing task. Changes in terminology, analysis methods, and the battery manufacturing process itself will need to be tracked and the ontology adapted. This includes formalizing the ontology and mapping it to other, more abstract ontologies such as EMMO, BattINFO, BVCO, and the ontologies of the German platform MaterialDigital (PMD) platform[37] to enable interoperability. Other, emerging ontologies that focus on process modeling are of interest as they provide different levels of abstraction for the production process and introduce control flow patterns beyond the sequential ordering realized here. We are considering the WiLD ontology,[38] which is based on a tree-shaped process representation,[39] for example. The extension and application phase will disencumber any geographical bias due to the fact that the workshops were done in Germany, despite the international background of most workshop participants and experts involved. There is a possibility that the English names for certain items/steps vary depending on the geographical location. Translations into other languages will be made through appropriate glossaries, if necessary. However, consensus on a universal digital vocabulary would be most effective.

The evaluation phase of the ontology engineering metaprocess will use the collected competency questions. Finally, the application and evolution phase of the ontology engineering meta-process will explore whether relational databases that are used to store data from reference battery production can be queried with the help of ontology-based data access methods,[40] e.g., via mappings from relational databases to RDF in R2RML[41] in SPARQL seamlessly with the PMD triple store(s).

The ontology will be provided to and released by PMD, enabling access to the community. While the proposed ontology was developed based on the reference process of the BLB, it has been abstracted sufficiently to be applied to different LIB production processes. It is suitable to identify and document differences in the underlying production process. Given the required expert knowledge, it is possible to add additional process steps, items, characterization methods, and properties. The structure based on items, steps, and characterization methods is abstract enough to be retained.

4. Experimental Section

The following section depicts the methods to develop the ontology for managing battery production and material data. The process of development consists of four main steps. First, a glossary covering all essential terms for the battery research field was created. Second, a reference process was captured in detail with all involved data structures and existing documents. Third, several interviews and workshops were conducted to define the terminology and decide on relevant information to be included in the ontology. Based on this information, competency questions were defined to define the scope of the developed ontology. Historical data helped in validating the created structure. Lastly, the collected data was used to develop the ontology covering the battery production process with the involved material.

Glossary: A predefined terminology is required to collect, combine, and structure the information necessary for the ontology. This is due to the complexity of the battery manufacturing processes and their involved materials. On the one hand, specific terminology, such as electrode, anode, and cathode, is well established and widely accepted. On the other hand, numerous intermediate products in the production process do not have a standardized term. To develop a broadly applicable ontology in battery research and manufacturing, every stakeholder and participant should share a common vocabulary. To this end, a glossary with names and definitions was established to prepare further steps. The collaborators on the present research project then used the terms defined in the glossary. This step also sets the basis for the terminology in the presented ontology.

Reference Process: To date, there is no universally applied standardized process for battery manufacturing established. While standardized processes within battery manufacturers and research institutions exist, they are differing from each other based on the company or institution. Even though the general procedure of battery cell production from the raw materials is comparable among different institutions and production scales, certain variations in material composition and process steps are possible.[21] Therefore, our approach in developing an ontology was to use a reference battery manufacturing process. An electrode and cell production process at the pilot plant BLB served as a viable reference process focusing on fundamental and application-oriented research questions. The developed ontology is based on the reference process as a prototype but will allow variations and adjustments if necessary.

Workshops: The stakeholders and involved partners in their field of expertise in different areas of the battery manufacturing process chain. To aggregate and combine existing information, thematic-specific workshops were carried out remotely (e.g. "electrode production processes", "analytical methods"). In total, eight workshops were conducted. In the first strategic and overarching structure workshops, up to ten participants including digitization and battery research experts were involved. In later validation workshops, up to 30 battery experts that are involved in German battery research clusters participated in addition to digitization experts. Already predefined questions were targeted and answered: 1) What is the scope of the developed ontology?; 2) What are the most important objects within the ontology?; 3) How can we combine the manufacturing process with the involved materials and their analytical characteristics?; 4) Which abstraction level allows space for variation and is at the same time specific enough to create value?

Competency Questions: While developing the ontology, main competency questions were formulated. Each competency question can be seen as a requirement that needs to be fulfilled by the ontology itself. The developed ontology should be able to answer the competency questions. 1) Which process steps are involved in our battery production process?; 2) Which process steps are generally used in most of the battery production procedures?; 3) Which items can be formulated as input items and output items of certain process steps?; 4) Which characterization methods can be applied to which items?; 5) Which properties does a given process step/item/characterization method require?; 6) Which characterization methods have been applied to which items?; 7) Which process instance contains a given property within a given range?; 8) Which units are used for a given property?

Usage of Existing Data Samples: Existing data samples resulting from the research projects MultiDis,[42,43] MiKal,[44] InTenZ,[45] DaLion,[46,47] FELIZ,[48,49] LiMaProMet[50] were tested on their applicability to the defined structure to verify the already gathered information. Two main aspects were taken into account: 1) Can all of the information in a data sample be mapped onto the defined structure?; 2) Assumed all information of a battery manufacturing process is mapped onto the defined structure, is the process itself linked to each available data creating a web of linked objects?

Development of a Graphical Representation of the Ontology: After verifying and adjusting the defined structure, the ontology was graphically depicted. The process was split into a sequence of process steps covering input and output items and internal process step properties. Every involved material and intermediate product contains properties. Over the whole ontology, every data point can be filled but does not need to be. With this strategy, the ontology user is not enforced but has the option to attach as much information to the process as necessary. The graphical representation can be seen in Section 2.3.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Keywords

battery production, battery research, cell production, data structures, electrode production, ontology, taxonomy

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