An Ontology for Selecting Inorganic Material Analytical Methods and Its Industrial Application*

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Abstract
This paper presents an ontology of analytical methods aimed at supporting the selection of appropriate methods for the analysis of inorganic materials. The selection of analytical *methods* and *instruments* should be made according to both the intended aim (hereafter *purpose*) and the requirements and constraints (*conditions*). Aiming such selection, we have built an ontology as a knowledge base based on an upper-level ontology YAMATO. An ontology-based system has been developed to assist engineers in selecting appropriate analytical methods based on specific analytical purposes and conditions. The system is implemented as a short-message-based interactive system, enabling users to systematically filter analytical methods according to the analytical conditions identified through interactive dialogue. Evaluation results demonstrate a high degree of accuracy in both the suggested methods and the filtering criteria provided during user interaction.

Keywords
Engineering, Decision Support, Analytical Methods, Inorganic Material

1. Introduction

In the manufacturing of inorganic materials, analytical methods play a critical role in investigating material properties and internal structures. In the context of Murata Manufacturing Co., Ltd (hereafter Murata) in this collaborative research, engineers in the analytical department (analytical engineer) are responsible for selecting appropriate analytical methods based on the intended aim (purpose) specified in request forms submitted by engineers from the manufacturing department (manufacturing engineer) as clients. For instance, for the purpose of detecting internal voids within a material, X-ray computed tomography (X-ray CT) and the Scanning Electron Microscope (SEM) are candidate methods. Among them, methods should be filtered according to several requirements and constraints such as non-destructiveness, high-resolutions, and X-ray-induced discoloration. It might be difficult for less experienced engineers to select a suitable method, taking into account such requirements. Since the manufacturing engineer as clients are often unaware of which material properties are critical for method selection, it is essential that these requirements be identified through interactive and explicit inquiry.

At the outset of the collaborative research, in Murata, an NLP-based system was proposed to analyze request forms for selecting suitable analytical methods. However, it was found by Murata that ambiguities in vocabulary definitions and levels of abstraction resulted in increased

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program complexity and diminished maintainability. Furthermore, since certain terms were often omitted or only implicitly stated in the request forms, a significant number of additional definitions were required, posing a major challenge to system development.

To address these challenges, this joint research project aims to develop an ontology-based recommendation system that suggests appropriate analytical methods for a given purpose taking requirements into account. The system employs a short-message-based interactive interface, allowing users to interactively filter candidate methods based on specific requirements. The primary focus of this research is to build an ontology that serves as an explicit and structured knowledge base for the system.

This paper is organized as follows. Section 2 outlines two key issues related to the ontology development. Section 3 reviews existing ontologies relevant to analytical methods. Section 4 presents the structure and content of the proposed ontology. Section 5 describes an evaluation of the ontology through its implementation in a prototype system, comparing its recommendations with past real-world analyses. Section 6 discusses the characteristics and advantages of the proposed ontology. Finally, Section 7 concludes the paper.

2. Research issues

The first issue lies in the fact that a single analytical method serves multiple purposes or aims. For instance, the Scanning Electron Microscope (SEM) may be used for various purposes such as analyzing surface morphology, detecting voids, or inspecting plating delamination. If all possible purposes are explicitly included in the definition of each method, the resulting ontology becomes overly complex and difficult to maintain when a new method is added. To address this, we propose a distinction between *analytical purpose actions* and *analytical actions*. The former corresponds to purposes specified in the request forms, while the latter represents generalized, multi-purpose atomic units of actions. *Analytical methods* such as SEM should be defined in terms of *analytical actions* rather than *analytical purpose actions*. By introducing *analytical actions* as intermediate types, the scale of definitions of analytical methods can be reduced, and the definitions can be reused more effectively within the ontology.

The second issue lies in the need to define a wide range of requirements and constraints in detailed and comprehensive manner in order to recommend appropriate *analytical methods* and *instruments*. For example, when recommending an X-ray CT, relevant requirements and constraints may include *density non-homogeneity* affecting X-ray CT accuracy, *discoloration* from X-ray exposure and the requirement for *non-destructive* analysis. These requirements and constraints are referred to as *analytical conditions* in this study. However, it is not always clear what these *analytical conditions* depend on, or to which qualities they should be attributed, and such interpretations may vary. Therefore, to ensure comprehensive and coherent definitions, it is essential to systematically define these *analytical conditions* while taking into account such ontological differences.

3. Related work and approach in this study

3.1. RadLex

In the field of radiology, the Radiological Society of North America has developed a taxonomy known as RadLex [1] specific to radiological practices. The analytical methods such as *Computed Tomography* and *Spectroscopy* are defined as sub-types within a hierarchical structure under *Imaging Specialty* → *Imaging Modality*, following a super-type → sub-type (*is-a*) relationship. While RadLex provides a unified taxonomy, prior studies have pointed out the importance of incorporating instrument-specific characteristics, such as the medium used for analysis (referred to as a probe), the analyzable properties, and the types of analytical results that can be obtained [2]. Accordingly, in this research, *analytical methods* are defined with a systematic structure that emphasizes the types of the probes (e.g., *X-ray* and *electron beam*) and the types of the analytical results (e.g., *transmission image* representing *internal morphology*).

3.2. SNOMED-CT

SNOMED CT is a taxonomy of medical terms [3], incorporating analytical methods such as *Computed Tomography* and *X-ray photon absorptiometry* within a hierarchical structure under *Procedure* ⟶ *Procedure by method* ⟶ *Evaluation procedure* ⟶ *Imaging* ⟶ *Radiographic imaging procedure*. Although developed primarily as medical terminology, various limitations have been identified when interpreted as an ontology [4]. This study addresses on one such issue: the use of the *is-a* relationship to represent the *purpose-means* relationship. For example, *Imaging* is defined as a sub-type of *Evaluation procedure*, implicitly suggesting that *evaluation* (purpose) can be achieved by (*diagnostic*) *imaging* (means). Our approach models actions related to analytical purposes (*purpose actions*) and the actions employed to achieve them (*means actions*) using a foundational construct: *role* [5][6][7] for more precise modeling.

3.3. Measurement Method Ontology

In the biomedical field, the Measurement Method Ontology was developed for integrating phenotypic measurement data [8]. Analytical methods are defined as sub-types under either *in vivo method* or *ex vivo method*; for example, *computed tomography* falls under *in vivo method* ⟶ *in vivo radiography* ⟶ *tomography*. While the ontology offers a comprehensive catalog of analytical methods, it lacks systematic classification based on *probe* types or *analytical results*. Our research proposes a structured classification of analytical methods based on these elements.

3.4. Characterisation Methodology Domain Ontology (CHAMEO)

The characterization methods and workflows for measuring material structures and properties have been ontologized in the Characterisation Methodology Domain Ontology (CHAMEO) [9]. Its important contribution includes the key steps in sample preparation and data post-processing. While the authors acknowledge the significance of these steps, the present study focuses on the measurement steps and considers only one type of preparation—namely, "cut a cross-section" as a preliminary step to "observe the surface" as described in Section 4.3.

4. Building an ontology of analytical methods

4.1. Overview of the ontology

The ontology built in this study conforms to an upper-level ontology YAMATO [10], albeit with partial simplifications. There are three primary reasons for adopting this upper-level ontology. First, YAMATO provides a framework for defining types in terms of roles [7][10], which is supported by the ontology editor Hozo [7][11]. Second, it offers a mechanism for explicitly describing the decomposition relations of actions through the *ways of achievement* as deployed in [12]. Third, YAMATO enables precise modeling of *information* as a role played by *representation* based on the systematic distinction between *form* and *content* [13].

The ontology was developed using Hozo and currently comprises 533 classes and 1,192 slots, which has been exported in both OWL and RDF formats. The term "slots" here refer to elements in frame-based knowledge representation, which roughly correspond to "properties" in RDF, constrained by "restriction" in OWL. The ontology has been developed based on literature related to analytical methods and instruments, provided by Murata and curated under the supervision of Murata's domain experts. The current ontology focuses mainly on observation of morphology and analysis of composition as analytical actions.

As illustrated in Figure 1, the main upper types in the ontology are: *analytical purpose action*, *analytical action*, *analytical method, analytical* instrument, and analytical condition. The recommendation system selects appropriate *analytical methods* based on the following relationship: "An *analysis method* **uses** an *analytical instrument*, whose **function** is an *analytical action* as a **partial function to achieve** the *analytical purpose action* described in the analytical request form. The **basic operation** of the *analytical method* is the *analytical action*, and the ***analysis constraint*** of the *analysis instrument* must be satisfied." The types shown in bold and indicated by arrows in Figure 1 are modeled in terms of **roles** [5][6][7].

4.2. Analytical action

An *analytical action* is defined as an atomic unit of action that cannot be further decomposed into partial actions (See Section 4.3). Analytical actions are broadly classified into three sub-types: "observe", "measure", and "process". Figure 2 shows the definition of the analytical action "observe internal morphology". In this definition, "what is to be analyzed by the action" (as for "target input object" and its quality) is specified as the "internal morphology" of an "object", while "what type of the analysis result is obtained" (as for "target output object") is specified as "transmission image" representing "internal morphology". In the Hozo ontology framework, the relationship between "target input/output objects" and the analytical action is represented by the *participate-in* relation (denoted as "p/i" in Figure 2).

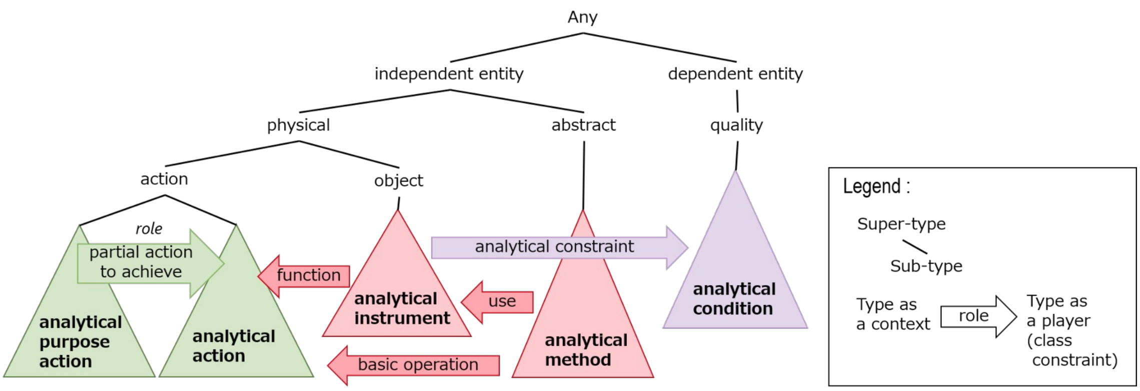

Figure 1: An overview of the ontology

In Hozo, the types are generally defined in terms of roles [7]. In YAMATO, roles are *anti-rigid*, *dynamic*, and *externally founded* [7]. A key principle is that a **potential player** for a **role** is a **role-holder** when it actually plays the role. A **role** is a dependent entity to be played, a **potential player** as a **class constraint** for the role slot is an entity that can play a role, and a potential player becomes a **role-holder** in playing a role. In the school example, when a person (a potential role player and a class constraint for the student-role slot) enrolls in a school (a context), the person plays the role of a student in the school and becomes a student (a role-holder, role-playing entity). The school example in Hozo is shown in the right of Figure 2. Such roles are represented as *qua*-classes, however, their *externally founded-ness* on the context might evoke the relational character typically associated with "properties".

As shown in the center of Figure 2, when "observing internal morphology" (a context), the **entity** to be observed is a physical "object" (a potential player/class constraint), which plays the role of "target input object" (a role/slot). The "object" become a role-holder "(target) input object" when it plays the role. The **quality** to be observed by this action is defined as "morphology" (as a potential player) playing "internal morphology"-role in a sub-slot.

The "transmission image" specified as a class constraint for the "target output object" slot in Figure 2 is defined in Figure 3 based on a theory of representation [13]. According to this theory, a *representation* consists of *representation form* and (*representation*) *content*[1], where a *representation-form* typically refers to an expression in some language as a sequence of symbols or to a visual form such as an image. In this case, the definition states that the *representation-form* of "transmission image" is an "image-form" (inherited from the class "visualization result of morphological observation") and the *content* is "internal morphology". In summary, when the action "observing internal morphology" is executed, a *representation* is generated as output whose *form* is "image" and *content* is the "internal morphology" of the target object.

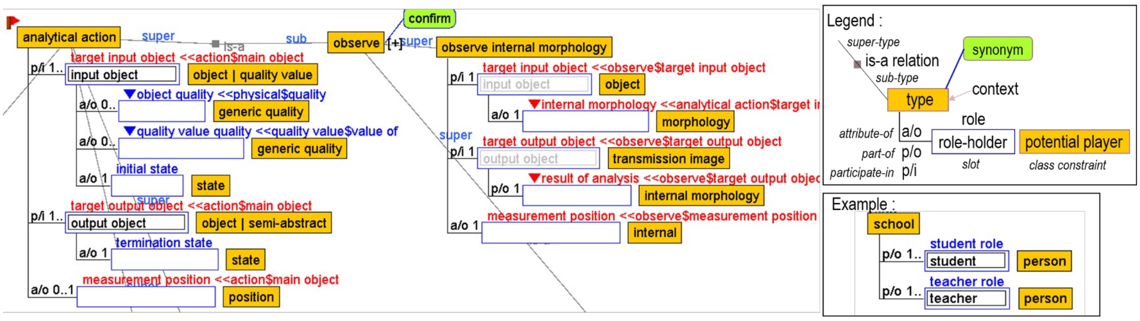

Figure 2: Definitions of "analytical action" and "observe internal morphology"

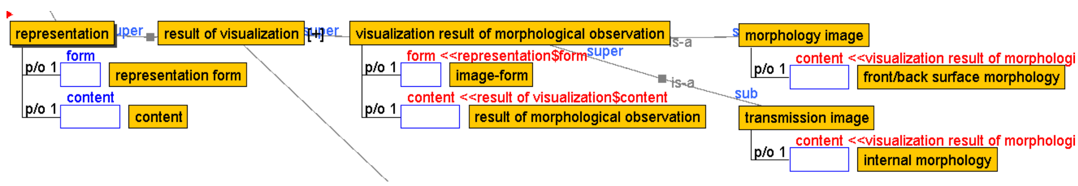

Figure 3: Definitions of "transmission image" as a "representation"

[1] Precisely speaking of [13], in addition, a *representing thing* is composed of a *representation* and a *representation medium*. For instance, a musical score (*representation*) consists of a sequence of musical notes (the *representation form*) and the specification of the sound sequence (the *content*); and a music book (the *representing thing*) is composed of some musical scores (*representations*) and some pieces of paper (*representation media*) where the musical scores are depicted. We do not consider *representing thing* or *representation media* here, as our focus does not require attention to physical *representation media* such as physical papers or digital files.

4.3. Analytical purpose action

An *analytical purpose action* refers to the aim of analysis, which are texts described in the analytical request form provided by the manufacturing engineers as clients. As represented by the *way of action achievement* [12] slot in Figure 4, an *analytical purpose action* can be achieved by one or more *analytical actions* (defined in Section 4.2) playing a role of **partial actions**. (More precisely, the class constraint is "analytical action | analytical purpose action" where "|" denotes a logical OR relationship.) For example, "observe void"—which aims to determine whether a void (i.e., a gap)[2] is present in a material—is defined in Figure 4. This action can be achieved in two different ways. In one way, referred to as the "way of directly observing the interior", it is achieved by a single partial (means) action: "observe internal morphology". In the other way, termed the "way of cutting a cross-section", it is achieved by two partial actions: "cut a cross-section" and "observe the surface" of the resulting cross-section. This approach allows *analytical purpose actions* to be defined as complex actions composed of *analytical actions*, which are treated as generalized building blocks.

4.4. Analytical instruments

An *analytical instrument* is primarily characterized by a "function" slot, whose class constraint is an *analytical action*, as well as by incident object ("probe") and detected object ("signal") slots, both constrained to "radiation | chemical substance". For example, the "X-ray computer tomograph instrument" (Figure 5) is defined as sub-type of "X-ray incidence analytical instrument", using "X-ray" as the probe. Its function slot is defined as "observe internal morphology", and its "analytical target object" slot is constrained to "void | individual object | component", representing the kinds of objects subject to analysis.

As discussed as the second issue in Section 2, each analytical instrument operates under specific conditions that the target object must satisfy. To represent such constraints, an "analytical constraint" sub-slot is defined within the "analytical target object" slot. For instance, the "X-ray computed tomography instrument" requires that the analytical target object possess a non-homogeneity density and that it does not undergo discoloration under X-ray exposure. These requirements are expressed in the analytical constraint slot as "density non-homogeneity" and "non-discoloration" (as discussed in Section 4.6), respectively, using the # operator, which indicates that the class itself rather than its instance is directly placed in the slot.

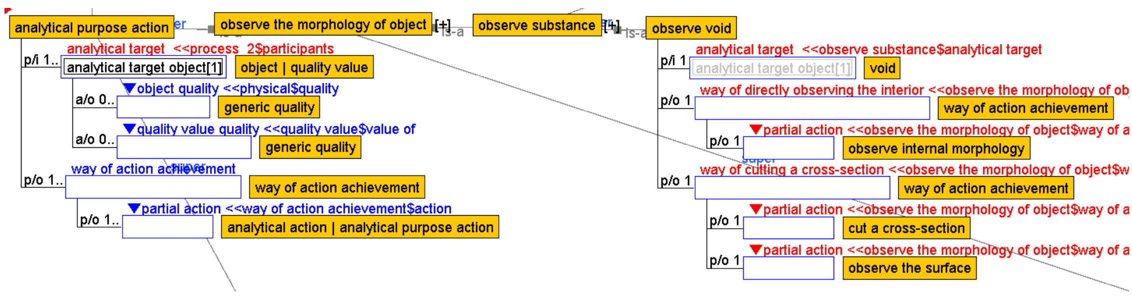

Figure 4: Definition of "analytical purpose action" and "observe void"

[2] Strictly speaking, a void like a "hole", is a "dependent entity" that lacks physical substance. In this study, however, it is treated as a sub-class of "physical objects" for simplicity.

4.5. Analytical method

An *analytical method* is primarily defined by the following slots: "basic operation", with a class constraint of *analytical action*; "usage analytical instrument", constrained by *analytical instrument*; and both probe and signal. For example, the "analytical method using incident X-ray" specifies "X-ray" as the class constraint in the *probe* slot (see Figure 6). Subsequently, the "X-ray computed tomography method" is defined by assigning the *analytical action* "observe internal morphology" (as described in Section 4.2 and Figure 2) to its *basic operation* slot.

This definition approach addresses the first issue discussed in Section 2. The X-ray computed tomography method is applicable to various *analytical purpose actions* (Section 4.3), such as "confirming deformation of void shape", " confirming the presence or absence of void", "measuring void size", and "analyzing failure". If each of these purpose-specific actions were directly specified to the *basic operation* slot, the number of slot definitions would increase significantly. By contrast, defining *analytical methods* in terms of generalized *analytical actions* as the *basic operation* reduces the definitional complexity. As a result, the total number of classes and slot definitions related to *analytical methods* was reduced by 55% compared to a model in which each *analytical purpose action* is directly linked to an *analytical method*.

In this study, the *basic operation* of an *analytical method* is defined to be identical to the *function* of the *analytical instrument* used in that method[3]. For example, the "X-ray computed tomography method" performs the action "observe the internal morphology", which corresponds directly to the *function* of the "X-ray computed tomography instrument".

4.6. Analytical conditions

As discussed as the second issue in Section 2, various kinds of *analytical conditions* influence the selection of methods and instruments. A*nalytical constraints* here as a sub-type of analytical condition refer to constraints on the qualities of the target object that affect instrument compatibility. These are classified under "target-object-related quality" and further divided into

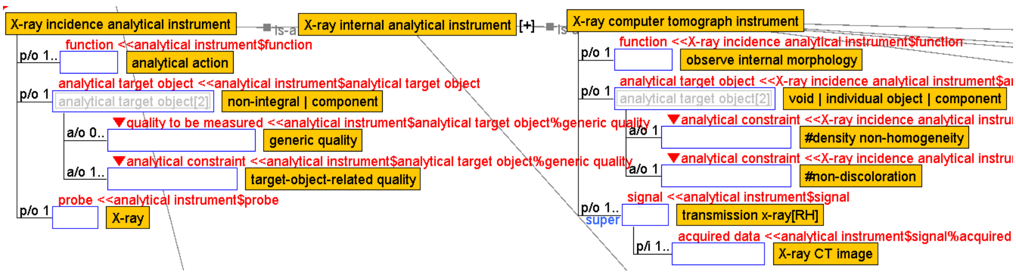

Figure 5: Definition of "X-ray computer tomograph instrument" with analytical constraints

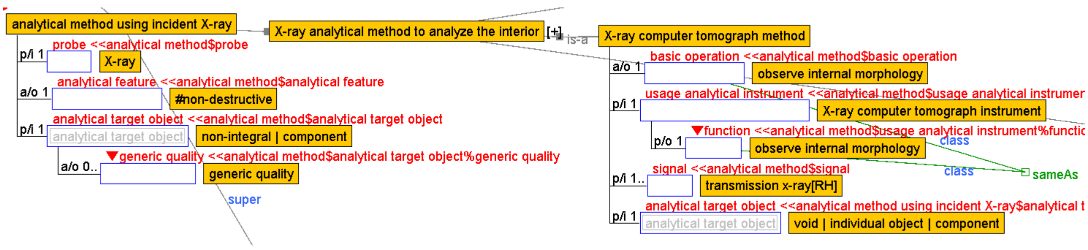

Figure 6: Definition of "X-ray computer tomograph method"

[3] Ontologically, *behavior* (including *actions/operations* here) and *function* are different. Roughly speaking, we define a function as a role(-holder) played by behavior of a device [14].

"analyzing-context-dependent quality" and "intrinsic quality of target object." A material quality falls into the former if its definition necessarily involves the environment of a specific instrument (*definitional dependency* in [5]), such as "non-discoloration" defined with reference to X-ray exposure in X-ray CT. The latter refers to intrinsic qualities defined without such reference to an instrument, such as "density non-homogeneity" which affects X-ray CT accuracy but whose definition itself does not necessarily involve the X-ray CT. These constraints are specified in the *analytical constraint* slot of *analytical instruments*, as discussed in Section 4.4 and shown in Figure 5.

In contrast, conditions such as the *non-destructive* nature of X-ray incidence analysis are not constraints on the target object but methodological features (referred to as *analytical features*) of the *analytical methods* themselves. Other examples include *low analysis accuracy* and *high compositional resolution*. These are defined under "analysis-related qualitative quality" and are specified in either of the *analytical feature* slot of *analytical methods* or the *quality* slot of *analytical actions*. For instance, "non-destructive" is specified as *analytical feature* for the "analytical method using incident X-ray," as shown in Figure 6, while "destructive" is specified for the "cut a cross-section" analytical action.

5. Implementation and evaluation of a recommendation system

5.1. A use case of a recommendation system

This section describes the recommendation system developed by Murata to support the selection of analytical methods by identifying the necessary conditions—information often implicit or insufficiently. The system uses a short-message-based interactive interface, allowing users to input required information by selecting from system-provided options. It employs the ontology defined using Hozo, exported into RDF format and queried via SPARQL. It does not employ so-called NLP-components but a simple short-text generation processing.

An example of the procedure for using the recommendation system—assuming a manufacturing engineer as the user—is presented below, based on an actual analytical request form: "Residue was found when creating a pattern in the etching process. Please confirm what are inclusions of the residue." Upon starting the system, the user is first presented with two alternative options for the analytical purpose: "observe morphology of objects" and "measure quality of objects". The two options are generated as a result of SPARQL query which retrieves direct sub-types of the *analytical purpose action,* which are always the same as the initial options. In this case, the user selects the latter, aiming to examine the composition of the residue.

In the second step, the user chooses "measure composition" out of five options. Subsequently, three more options are displayed: "measure difference of composition", "confirm presence or absence of an element", and "end of selection". Since the option "measure composition" selected in the second step is already appropriate, the user selects "end of selection". Through this three-step interaction, the system enables the user to specify the *analytical purpose action* in a guided and incremental manner.

Next, at the fourth step, the system displays possible ways to achieve the selected "measure composition" action. In this example, only one option—"way of composition measurement"—is presented and subsequently selected by the user. In cases where multiple ways exist to achieve a given action—such as "observe void", as described in Section 4.3—the system displays all applicable options, allowing the user to select the most appropriate approach.

At the fifth step, the system presents the *analytical actions* required to realize the specified *analytical purpose action* via the selected *way of achievement*. In this example, only one action —*"measure composition"*—is displayed and subsequently selected. In other cases—such as the *"*observe void*"* action—multiple *analytical actions*, such as "cut a cross-section" and "observe surface" of the resulting cross-section, may be required and are presented accordingly as necessary actions for achieving the specified purpose.

As the sixth step, the system retrieves *analysis methods* that have "measure composition" specified as *basic operation*. As a result, the five methods are enumerated as candidates such as "Energy-Dispersive X-ray Analysis (SEM-EDX)", " Wavelength-Dispersive X-ray Analysis (WDX)", and "X-ray Fluorescence Analysis (XRF)".

The subsequent steps involve filtering the candidate methods. The first question presented is *"*What is the kind of the target sample?"*,* accompanied by a list of selectable options. In this example, the user selects *"*powder*"* as the sample type. Next, the system presents a question whether the sample is heat-resistant up to 300°C. In this example, "yes" is selected, as the sample is inorganic residue in the etching process. Subsequently, a question concerning the required detection sensitivity is displayed, with the following options: "0.1% ~", "0.5% ~ 1%", and "Unknown". In this case, the user selects "Unknown".

Based on the responses provided, the system filters inappropriate candidate methods and recommends SEM-EDX and WDX as appropriate analytical methods. The suitability of this recommendation has been confirmed by domain experts.

5.2. Evaluation of the Ontology and the System

The evaluation of the system was conducted manually using a private database in Murata of real-world analytical case documents, which included both analysis requests and corresponding analysis reports. The total number of cases in the database was 110,028 (denoted as A). From this dataset, cases that fall within the scope of the ontology were extracted for evaluation, resulting in a subset of 16,603 cases (denoted as M). For instance, documents related to the measurement of thermophysical properties or structural analysis were excluded, as these analytical domains are not yet defined within the current ontology. From the target subset (M), a sample of 163 cases (denoted as N) was randomly selected and evaluated as described below.

First, the items and descriptions of each sample were extracted from the corresponding analysis request documents. Next, the system was operated following the procedure described in Section 5.1. The system was then evaluated based on the criteria listed in Table 1. Each evaluation item was scored on a scale of 0 to 10, according to the proportion of appropriate elements either defined in the ontology (for ontology evaluation) or correctly output by the system (for system evaluation). For example, in the case of Item No. 2.1 in Table 1, if five filtering conditions were deemed necessary but one was missing, a score of 8 out of 10 was assigned, as 4 out of 5 required elements were appropriately handled.

The evaluation was designed to distinguish between issues attributable to the system implementation and those arising from the ontology definition. For instance, if the ontology is correctly defined but the system fails to produce the correct output due to a program error, the scores for the ontology and system will differ accordingly.

The evaluation results are summarized in Table 1. For the ontology evaluation, each item received a high score of 9.9 or above. Similarly, for the system evaluation, all items scored 9.5 or higher. The overall average score across all evaluation items was 9.9, indicating that the developed ontology and system are generally capable of appropriately processing analysis requests found in the real-world case database.

Table 1
Evaluation items and results.

Phase	Item No.	Evaluation Item	Evaluation Score	
			Ontology	System
Pre-processing: Candidate Extraction	1.1	Are the necessary branches and options for selection available?	9.99	9.95
	1.2	Are the meanings of the options clear? (Was it necessary to revisit and revise selections?)	9.98	9.75
Post-processing: Candidate Filtering	2.1	Are all necessary filtering conditions present?	9.90	9.51
	2.2	Were the analytical methods filtered appropriately? (Are any clearly inappropriate methods included?)	9.97	9.88
	2.3	Are there any issues in filtering when the answer "unknown" is selected?	10.00	10.00
	2.4	Is the proposed method overqualified or exceeding the required specifications?	10.00	10.00

5.3. Prospects

The mean score obtained from the sample data was 9.910, and the lower bound of the 95% confidence interval was calculated to be 9.788. This result indicates a consistently high level of performance, even when considering the full evaluation target set (M). Therefore, it can be expected that the remaining cases in the dataset M can also be appropriately processed.

Of the 110,028 total cases (A), 16,603 cases (M)—approximately 15%—were classified within the current ontology scope. While this is a small fraction, the domain experts regard the ontology's structural design as sufficiently general and robust to cover the remaining 85% of cases. Therefore, future extensions are expected to involve primarily additive rather than structural changes, requiring significantly less effort than a linear 85%-to-15% extrapolation might suggest. With targeted modifications and incremental additions, the system is expected to be ready for practical deployment.

The major aspects currently outside the current scope—namely, sample preparation and post-processing—are acknowledged, as discussed in Section 3.4. Similar to the currently defined action "cut a cross-section", other pre- and post-processing actions could also be accommodated.

6. Discussion

The developed ontology incorporates two key features. First, user-input *analytical purpose actions*—such as "observing voids" (Section 4.3)—are decomposed into *analytical actions* like "cutting a cross-section" and "observing the surface" of the cross-section (Section 4.2). *Analytical methods*, such as "X-ray CT method" (Section 4.5), are then defined in terms of these *analytical actions*, which serve as the intermediate bridging types. As a result, the number of slot definitions was reduced to 55% compared to an alternative approach that defines *analytical methods* directly in terms of *analytical purpose actions* for the first issue identified in Section 2.

The second feature of the ontology is the systematic definition of *analytical conditions*, addressing the second issue in Section 2. This study distinguishes between (1) *analytical features* of *analytical methods* or *actions* (e.g., the non-destructive nature of X-ray incidence analysis) and (2) *analytical constraints* on target materials for specific *analytical instruments*. Item (2) is further divided into (2-1) analyzing-environment-dependent qualities (e.g., non-discoloration in X-ray CT) and (2-2) intrinsic qualities (e.g., density non-homogeneity affecting X-ray CT accuracy). These are systematically specified in the *analytical feature* slots of *analytical methods* or *actions* (item (1)) or the *analytical constraint* slots of *analytical instruments* (item (2)).

In comparison with existing ontologies such as RadLex, SNOMED-CT, and the Measurement Method Ontology (as summarized in Section 3), the ontology developed in this study provides a more expressive and functionally rich framework. *Analytical methods* are explicitly classified by probes and signals, such as X-rays and electron beams. In addition, the ontology introduces *is-achieved-by* relationships to represent the linkage between *analytical purpose actions* and *analytical actions*, thereby making a clear distinction from the *is-a* hierarchy. The analytical conditions as well are sufficiently defined as demonstrated by the evaluation.

In recent years, recommendation systems utilizing large language models (LLMs) have been actively developed [15]. However, when a general-domain LLM is employed for recommending analytical methods or analytical report documents are given to an LLM as domain-specific resources in the retrieval-augmented generation (RAG) architecture [16], there is no guarantee that all necessary conditions are consistently or explicitly described, as these documents often contain incomplete information regarding analytical purposes and conditions. When the system displays insufficient conditions in user interaction then the user inputs conditions insufficiently, this might lead to inappropriate recommendations. For instance, among the several selecting conditions for the X-ray CT method, the discoloration is not identified by Open AI's GPT-4-turbo (as of April 2025) as a relevant condition unless the user explicitly specifies it. In this study, analytical conditions are systematically formalized within an ontology, allowing the system to query users for the necessary conditions, as demonstrated by the evaluation. While an ontology could be incorporated into an LLM framework through the RAG (for example, the knowledge-graph RAG in [17]), by combining it with the system's ability to query users for necessary conditions, it can be used in a more conversational and natural dialogue format than the current implementation. In this context, the ontology itself remains an essential component.

The developed ontology, the implemented system and the used database through this collaborative work are the joint and proprietary intellectual property of Murata and Ritsumeikan University. Portions of the ontology contain Murata's trade secrets. Therefore, the full content cannot be made publicly available. While we acknowledge the importance of the FAIR principles, this paper aims to share the major design decisions underlying the ontology.

7. Concluding remarks

This paper presents an ontology of analytical methods for inorganic materials and its application in a recommendation system. The evaluation results demonstrate that the ontology appropriately supports method selection, particularly by incorporating analytical conditions. Currently, the ontology covers approximately 15% of the analytical records from past analyses conducted within an industrial setting. However, domain experts estimate that extending the ontology to cover the remaining 85% will primarily involve the addition of new analytical methods, without requiring modifications to the underlying structure. Based on this extensibility, the system is expected to be applicable to practical operations.

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Declaration on Generative AI

During the preparation of this work, the authors used ChatGPT, in order to: Grammar and spelling check, Paraphrase and reword, Text Translation. After using this tool/service, the authors reviewed and edited the content as needed and take full responsibility for the publication's content.

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