# A metadata schema for documenting material samples from multiple domains


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# A metadata schema for documenting material samples from multiple domains

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**Abstract.** This paper documents a metadata schema, implementation, and associated vocabularies developed for the Internet of Samples (iSamples) project to integrate geoscience, archaeology/anthropology, biology and genomics sample descriptions in a single cross-domain catalog. To develop the sample description scheme for sample discovery across these disparate domains, we reviewed the metadata schema and example metadata from each project partner, as well as other existing schemes. Top level classes in the schema include MaterialSampleRecord, Curation, SamplingEvent, SamplingSite and Agent. By factoring sample type classification into material type, material sample object type, and sampled feature type, it has been possible to classify the approximately 6,000,000 samples in the combined corpus. Category vocabularies for these classifications were developed based unique value summaries from related fields in the source sample metadata, tested using a card sorting exercise and by development of code for automated mapping from source metadata. Each vocabulary has on the order of 20 categories with some hierarchy; the category concepts are intended to be covering, but might overlap. These vocabularies are implemented in SKOS, and published with the ARDC Research Vocabularies Australia (RVA) vocabulary service. The metadata schema is defined using a LinkML YAML file, and implemented as a JSON schema used to validate instance documents. To support interoperability mapping from the iSamples metadata schema to several other schemes is provided in the project Github.

Keywords: material sample, metadata, interoperability, cross-domain

## 1. Introduction

The Internet of Samples (iSamples) project, funded by the U.S. National Science Foundation, is working to enable connections between diverse data derived from material samples across science domains to facilitate interdisciplinary collaborations. The project brings together sample collection and data repository managers from the System for Earth Sample Registration (SESAR)[1], Open Context (a publishing service maintained by the Alexandria Archive Institute, a metadata repository for archaeological artifacts and ecofacts)[2], the Genomic Observatories Meta-Database (GEOME)[3], and Smithsonian Institution Museum of

1 https://www.geosamples.org/
2 https://opencontext.org/

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3 https://geome-db.org/

Natural History (NMNH)[4], representing geoscience, archaeology / anthropology, and biology / genomics disciplines. The goal is a searchable index of material samples described by rich metadata and linked to derived research products. iSamples aims to (i) enable connections between diverse and disparate information derived from material samples; (ii) support existing research programs and facilities that collect and manage diverse sample types; (iii) facilitate new interdisciplinary collaborations; and (iv) provide an efficient solution for FAIR samples, avoiding duplicate efforts in different domains.

To achieve these goals, iSamples must incorporate and help advance development and adoption of metadata vocabularies and content standards across science domains. As a starting point, we have developed a core sample description scheme applicable to material samples from any of the partner systems. Our approach to developing the schema was empirical, based on reviewing existing sample description schemes in use (Table 1) and on reviewing the content in the metadata records from project partner systems to evaluate what fields are populated.

Table 1. Existing systems with some material sample description model.

| System | Name | Notes |
|---|---|---|
| IGSN | International Generic sample Number | originally focused on Earth Science material samples, then expanded to register other kinds of samples. Original design had very simple 'registration' scheme and more in depth descriptive scheme that could be extended for different sample types[5,6]. IGSN is now incorporated into the DOI system under the authority of DataCite, and uses the DataCite metadata schema. |
| GeoSciML[7] | Geoscience markup language | XML implementation based on a conceptual model for geologic data. Model is presented using UML. Material samples are modeled as a kind of sampling feature[8] based on the OGC Observation and Measurement model. |
| ODM2[9] | Observation data model | Entity relation model developed by the Critical Zone Community, similar to OGC Observation and Measurement model; treats material sample as 'specimen', a kind of sampling feature[10]. |
| TDWG-MIDS | Biodiversity Information Standards Minimum Information about a Digital Specimen | Basic content model for a metadata record describing a material sample [4] |
| SESAR[11] | System for Earth SAmple Registration | US Node in IGSN network; extends IGSN metadata schema with additional content[12]. |
| W3C SSN[13] | World Wide Web Consortium activity developing an ontology for sensor networks; | Sample and sampling activity are included in the model[14] |

4 https://naturalhistory.si.edu/research

5 https://igsn.github.io/metadata/, https://github.com/IGSN/metadata

6 https://archive-intranet.ardc.edu.au/display/DOC/IGSN+Descriptive+Metadata

7 https://geosciml.org/

8 see https://docs.ogc.org/is/16-008/16-008.html#357 and https://docs.ogc.org/is/16-008/16-008.html#443

9 https://github.com/ODM2/ODM2

10 https://github.com/ODM2/ODM2/blob/master/doc/ODM2Docs/ext_samplingfeatures.md#sampling-features-that-are-specimens; https://odm2.github.io/ODM2/schemas/ODM2_Current/tables/ODM2SamplingFeatures_Specimens.html

11 https://www.geosamples.org/

12 https://zenodo.org/doi/10.5281/zenodo.3875530

13 https://www.w3.org/TR/vocab-ssn/

14 https://www.w3.org/TR/vocab-ssn/#SOSASample

| System | Name | Notes |
|---|---|---|
| ESS-DIVE | Environmental System Science Data Infrastructure for a Virtual Ecosystem | ESS-DIVE Sample ID and Metadata Reporting Format (IGSN-ESS)[15] |
| DISSCo[16] | Distributed Systems of Scientific Collections | DiSSCo specimen & collection classification. Focused on digital representation of material samples, and linkage to related resources[17]. |

Another important source for developing the schema is a metadata cross walk document prepared in conjunction with research for [2], and shared with the iSamples team by J E. Damerow (Personal Comm). Results from several workshops over the last several years have also be used; these include workshops to develop the basic and description metadata for International Generic Sample Number (IGSN), and to review the material sample metadata for the USGS National Geological and Geophysical Preservation program. In the context of this work, we are interested in material samples. These are material entities collected and identified with the intention of being representative of some feature of interest in the world[18]. The term 'sample' as used in this document should be understood to mean such a 'material sample'.

Categorization of sample type is an attribute typically included metadata systems for describing samples. In most cases this categorization is done with a controlled vocabulary to provide a means to zero in on kinds of sample a user is looking for. We reviewed the sample type classifications used in the metadata corpus from the project partners and determined that a single sample type classification vocabulary could not account for the spectrum of samples without becoming too large and unwieldy. By factoring sample type categorization into material type, material sample object type, and sampled feature type, it has been possible to classify the approximately 6,000,000 samples in the combined corpus. Material Type specifies the kind of substance that constitutes the sample, for example 'Rock', 'Organic material', 'Liquid water', 'Anthropogenic material'. Material Sample Object Type specifies the kind of physical object identified as the sample, for example 'Fossil', 'Artifact', 'Organism part'. Sampled Feature Type specifies the thing in the world the sample is intended to represent, for example 'Site of past human activity', 'Atmosphere', 'Extraterrestrial environment'. These vocabularies are briefly presented below, and can be viewed in more detail at web pages from the project GitHub[19].

This paper first describes an information model for the content of a material sample description. Next the vocabularies for documenting sample type are described, followed by a discussion of the physical implementation of the information model. The final section briefly summarizes testing of the metadata schema for integration of sample descriptions from the project partners.

## 2. Sample description information model

The information model for the material sample description scheme defines the content items used to describe a sample. Only the most critical items are made mandatory. The physical implementation used for the iSamples catalog is described in a subsequent section.

### *2.1. Registration metadata*

Registration metadata includes information about the sample description (metadata) record itself and is useful for management of the metadata in a distributed information system such as is envisioned for the iSamples architecture [7].

#### *2.1.1. Metadata identifier*

This is an identifier for the metadata record, distinct from the identifier for the physical object the metadata documents. Dereferencing[20] the *Sample identifier* (see following section) will typically return information from the metadata record describing the sample and is thus commonly confused with the *Metadata identifier*

[15] https://github.com/ess-dive-community/essdive-sample-id-metadata
[16] https://dissco.tech/2020/03/31/what-is-a-digital-specimen/
[17] https://docs.google.com/document/d/19OPyOm9VF2qfI3M6Rm
[18] https://dwc.tdwg.org/list/#dwc_MaterialSample, http://www.opengis.net/doc/as/om/3.0
[19] https://isamplesorg.github.io/models/
[20] Dereferencing is the process of retrieving information about the entity (resource) that an identifier represents.

(Figure 1). The material sample and the metadata record are considered separate resources. A distinct identifier for the metadata record allows statements to be made (annotation) about the metadata record, for example to make corrections, point out errors, or add links to new resources.

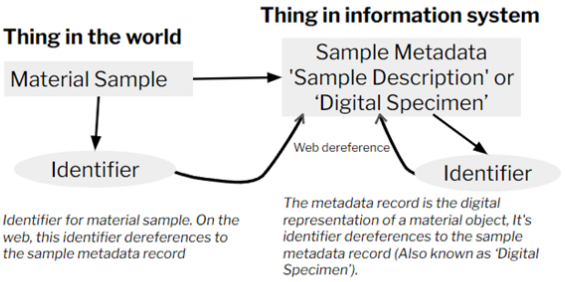


Fig. 1. Relationship between the material sample and its representation in the digital information system.

*2.1.2. Registering agent*

This identifies the agent, a person or organization, responsible for the metadata record. Having contact information for the agent included is important to enable harvesters or other users to notify the metadata originator about problems or suggest updates and improvements to the sample metadata content. The agent should be specified with a name for human use to identify the agent, a resolvable URI to identify the agent in a linked data context, and a point of contact address or phone number. ORCIDs are recommended for persons and ROR identifiers for organizations. An institutional role e-mail is recommended as a point of contact address, e.g. 'sampleCurator@AcmeUni.edu', as these are less likely to go stale when staffing changes occur.

*2.2. Basic discovery metadata*

The following properties are considered mandatory for a basic sample description supporting discovery and resolution of sample identifiers (Figure 2).

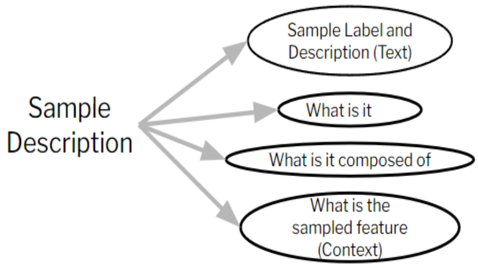


Fig. 2. Questions addressed by basic discovery metadata.

*2.2.1. Sample Identifier*

This is a string that uniquely identifies the material sample. It should be a persistent, web-resolvable URI (e.g. an http URI). iSamples project participants are using ARK (Archival Resource Key) identifiers and IGSN[21] identifiers. The material sample is a physical entity and cannot be transmitted electronically. The iSamples metadata record is considered the default electronic representation of the physical entity. The material sample has an identifier, ideally attached to the physical entity; when this identifier is dereferenced electronically (on the web) the default electronic representation is provided as a proxy for the physical entity (Figure 1). The metadata record is the anchor for the 'Digital Specimen' network of linked data about the material sample. It has a separate identifier from the material sample, allowing statements to be made about the metadata distinct from statements about the material sample.

*2.2.2. Label*

A text string that identifies the sample for human users. In many cases this is an identifier string assigned by the original sample collector. Other identifiers or labels assigned to the sample can be recorded in the alternate identifier field (see below).

*2.2.3. Alternate identifiers*

This item contains other identifiers used to represent the sample. These might include a field identifier assigned by the sample collector, laboratory-assigned identifiers used in analysis workflows, or museum accession numbers. The identifier string value should be accompanied by a scheme name to identify the scope in which the identifier is used and assumed to be unique.

[21] IGSN identifiers are now issued by Data Cite and conform to the DOI scheme. See https://support.datacite.org/docs/igsn-faq.

*2.2.4. Description*

A free text description of the sample. This text will be indexed by search applications and read by users to understand what the sample is. More information is better. The description should include how and why the sample was collected, any particulars of the collection context, and a physical description of the sample-size, mass, color, material composition, etc. Cryptic abbreviations and acronyms, as well as project- or domain-specific jargon should be avoided.

*2.2.5. Sample type: Material type, Material sample object type and Sampled feature type*

Samples can be categorized in various ways. After reviewing example metadata from project participants, it was determined that factoring sample type into three properties: material type, material sample object type and sampled feature type provides an effective scheme that can be implemented with ~20 classes in each property vocabulary. These properties answer the basic questions about the sample: what is it composed of?, what is it?, what does it represent? The vocabularies are described in more detail and listed in the vocabulary section, below.

*2.3. Additional important information*

These properties are not essential for basic discovery, but useful to enable access and reuse, and to fully implement the FAIR principles for material samples (Figure 3).

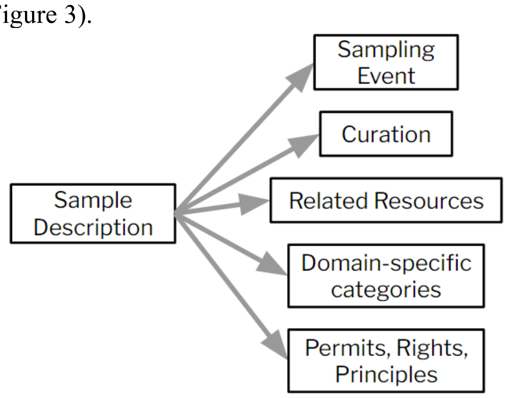


Fig. 3. Other sample description elements

*2.3.1. SamplingEvent*

A sample is the product of a sampling event. Documentation of the sampling event comprises subitems that specify where and when the sampling took place, what was sampled, how the sampling was done, any conventions, protocols, or policies followed in sample collection, permissions obtained for sampling, and who did the sampling. These aspects are elucidated below.

*Where:*

For many samples, the location where the sample was collected provides important information for data integration and understanding the sample context. Location can be specified at different levels of resolution, ranging from a general place name to a very specific location in a high-resolution local coordinate system like a survey grid at an excavation. Reporting the location with latitude and longitude coordinates in decimal degrees with 2 to 4 decimal places precision using the WGS84 coordinate reference system is required for ease of use and comparison to sample locations reported from different collections. Locations using other reference systems, e.g. site-specific grids or linear reference like depth in a non-vertical borehole, should be described in the sampling site description as free text. Be sure to include description of the coordinate reference system used.

If access to the sampling location or removal of material from the location required one or more permits, information about permits obtained for access and sampling should be included in the authorized_by property. Sampling locations might also be approximated to avoid abuse; the metadata scheme includes a field ('obfuscated') to indicate if the location is intentionally approximate.

*Procedure*

The sampling procedure or protocol should be documented as a property of the sampling event. The procedure might be specified with a text description, or if it is formally documented with an identifier (e.g. protocols.io[22]), a label and identifier should be provided.

*Sampling event responsible parties*

The parties responsible for the sample collection event should be acknowledged in this section. 'Party' can be a person or an organization. Each party has a role such as collector or funder that specifies their relationship to the sampling event. Role names from a controlled vocabulary should used, but this specification does not specify a particular vocabulary; ISO19115 Role Codes[23] or the Contributor Role Ontology [9] are suggested for use. A name must be

[22] https://www.protocols.io/

[23] https://wiki.esipfed.org/ISO_19115-3_Codelists#CI_RoleCode

provided for each party. Organization affiliation can be specified for persons. Each party should have a persistent, resolvable identifier to support data integration and interoperability. The use of ORCID[24] to identify persons and ROR[25] to identify organizations is recommended.

### 2.3.2. Curation and access

The curation and access description documents where the sample is currently located, how it has been preserved or otherwise modified, procedures to access the sample, and constraints on usage of the sample.

In analytical chemistry, sample preparation refers to the ways in which a sample is treated prior to its analyses.[26] For biological samples (and some other types) the 'Preparation' or preservation method is an important consideration. In Darwin core 'preparations'[27] is defined as 'A preparation or preservation method for a dwc:MaterialEntity [material entity]'. For iSample purposes, we consider curation to be the set of activities between when a sample was originally collected and assigned an identifier and its current state. These activities might include various preservation steps to stabilize the sample in its original state. Preparation is the subset of curation activities specifically focused on changes to the sample necessary to support some analytical activity.

Use of a controlled vocabulary to describe sample processing would help search precision for use cases when sample processing is a filter criteria. One possible vocabulary is the Sample Processing and Separation Techniques Ontology[28], and projects are under way to develop conventions in the Biomolecular Ocean Observing and Research community [8]. Description of curation activities in text will assist users in evaluating the fitness of a sample for reuse purposes.

*Curation responsible parties*

The parties responsible for curation of the sample should be acknowledged in this section. 'Party' can be a person or an organization. Each party has a role such as curator, collections manager or analyst. Role names from a controlled vocabulary should be used, but this specification does not specify a particular vocabulary. A name must be provided for each party; organization affiliation can be specified for persons. Each party should have a persistent, resolvable identifier to support data integration and interoperability. The use of ORCID[29] to identify persons and ROR[30] to identify organizations is recommended. At least one party should be identified as the point of contact if the sample is available for viewing or possible loan, with included contact information.

*Storage location*

The location where the sample is physically stored should be identified at the organization or facility level, if known or applicable. Details about specific shelf or drawer is useful for collection curators, but not necessary for sample search and evaluation.

*Access and usage constraints*

Any restrictions or policies that determine whether or how the sample may be viewed or borrowed should be explained in the metadata. If the access and usage policies are defined in online documents, URLs to access those documents should be provided.

### 2.3.3. Domain-Specific Categories: Keywords

Keywords are not required but are recommended. They are useful for providing other categorization or descriptive words to make discovering and evaluating a sample more accurate. The three iSamples sample type vocabularies are very high level and need to be supplemented by keywords that categorize the material sample in more domain-specific terms. The keyword implementation allows for a keyword term, keyword identifier, keyword scheme name and scheme identifier. The keyword term is the minimal requirement; if no identifier or keyword scheme is provided the term is treated as a simple 'tag'—a word or phrase that expected users might associate with the sample. If the keyword is from a controlled vocabulary with more precise semantics and can be used for cross-domain searches, the keyword identifier, scheme name, or scheme identifier should be provided. Keywords from controlled vocabularies can be used to associate other categorical property values with the sample, e.g. geologic age, biological taxonomy classification, or archaeologic material culture, using the scheme name to specify the property.

### 2.3.4. Related Resources

To take advantage of the linked data capabilities of the World Wide Web, it is useful to provide links to related resources for understanding the sample,

[24] https://orcid.org/
[25] https://ror.org/
[26] https://en.wikipedia.org/wiki/Sample_preparation
[27] https://dwc.tdwg.org/list/#dwc_preparations
[28] https://bioportal.bioontology.org/ontologies/SEP
[29] https://orcid.org/
[30] https://ror.org/

discovering data derived from the sample, or finding related research. The most important relationship to report is linkage between parent and child samples. Other related resources include publications or datasets using data from the sample, and collections in which the sample is a member. Links to related resources should include a resolvable identifier (e.g. an http URI) for the target resource, a label for the link, and a relationship type term from a controlled vocabulary to categorize the nature of the relationship. A sample relationship type vocabulary is in development.[31]

#### *2.3.5. Permits, Rights, Principles*

The sample metadata includes properties to specify legal, cultural, or policy considerations or constraints that might be critical to enable use of the sample and derived data. As mentioned in the Sampling event section (above), permits that provide permission to access sampling locations or remove material should be cited in the 'authorized_by' property on the sampling event. Restrictions on access to or use of the sample can be specified in the 'dc_rights' property on the sample. Conformance with other policies and procedures, e.g. those related to the CARE Principles[32] [1], can be asserted using the 'complies_with' property on the sample. These metadata fields currently contain string values, allowing text descriptions, or links to documents or other resources.

### *2.4. Other Properties, Domain Specific Categories and Contexts*

There are a variety of other properties that are important for samples in some domains, for example dimensions, mass, origin age, rock type, mineral type, biological taxon, tectonic setting, archaeological culture, or biome. If such properties have categorical values, they can be asserted in the sample descriptions as keywords (see Domain-Specific Categories: Keywords). In version one sample description implementation for iSamples, properties with numeric values should be summarized with text statements in the sample descriptions. This will make the information available to human users. The text will be indexed as free text for search, but the results will be somewhat unpredictable because the information is not structured. We envision future development of extension profiles to define structured and interoperable scheme for assigning such properties.

## 3. Vocabularies

A single classification vocabulary for sample types cannot account for the spectrum of possibilities in the project scope without becoming very large and unwieldy. By factoring the categorization into material sample object type, material type, and sampled feature type, it has been possible to classify the approximately 6,000,000 samples in the combined corpus. Material type specifies the kind of substance that constitutes the sample, for example 'Rock', 'Organic material', 'Liquid water', 'Anthropogenic material' (Figure 4). Material sample object type specifies the kind of physical object identified as the 'sample', for example 'Fossil', 'Artifact', 'Experiment product', 'Organism part' (Figure 5). Sampled feature type specifies the thing in the world the sample is intended to represent, for

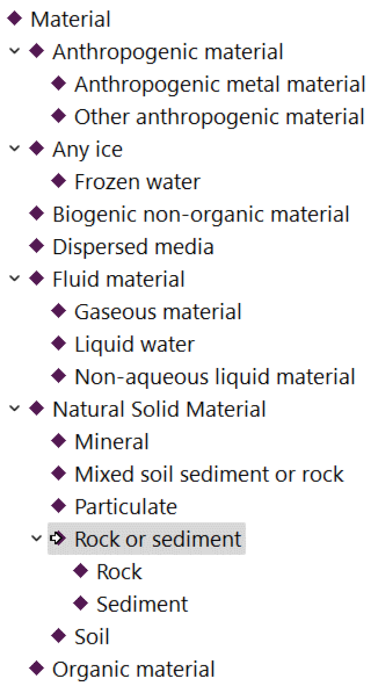


Fig. 4. Hierarchical relationships between material types.

[31] https://bit.ly/isamples-relationshipscv

[32] https://www.gida-global.org/care

- Material sample
  - Any aggregation material sample
    - Aggregation
    - Anthropogenic aggregation
    - Biome aggregation sample
  - Biological material sample
    - Biome aggregation sample
      - Bundle biome aggregation
      - Slurry biome aggregation
    - Organism part
    - Organism product
    - Whole organism material sample
  - Fluid in container
  - Non biologic solid object
    - Artifact
    - Fossil
    - Other solid object
    - Solid material sample
  - Research product
    - Analytical preparation
    - Experiment product

Fig. 5. Hierarchical relationships of material sample object type terms.

- Any sampled feature
  - Anthropogenic environment
    - Active human occupation site
      - Experiment setting
      - Laboratory or curatorial environment
    - Site of past human activities
  - Biological entity
  - Earth environment
    - Atmosphere
    - Earth interior
    - Earth surface
      - Lake river or stream bottom
      - Marine water body bottom
      - Subaerial surface environment
    - Glacier environment
    - Subsurface fluid reservoir
    - Water body
      - Marine environment
      - Terrestrial water body
  - Extraterrestrial environment

Fig. 6. Hierarchical relationships of sampled feature types.

example 'Site of past human activity', 'Atmosphere', 'Extraterrestrial environment' (Figure 6). Full listing of the vocabularies with definitions can be found at the iSamples web site[33] or the ARDC Research Vocabularies web site[34]. High-level vocabularies were developed based on unique value summaries from related fields in the source sample metadata. The draft vocabularies were tested with the project team using a card-sorting exercise, and by developing code for automated mapping from source metadata to iSamples metadata. Our goal was that each vocabulary should have around 20 values, have some hierarchy, and should cover the range of possible values. Vocabulary concepts are possibly overlapping, such that some samples might be categorized in more than one class.

The vocabularies have been implemented in Resource Description Framework (RDF)[35] using the Simple Knowledge Organization System (SKOS)[36] vocabulary. Each concept has a Uniform Resource Identifier (URI)[37], preferred label, and a definition; notes and examples are included for some concepts. Hierarchical relations are represented using skos:broader. Where mapping to concepts in other vocabularies has been found, relationships are represented using one of the SKOS mapping relations: broadMatch, narrowMatch, closeMatch, exactMatch. The vocabularies are defined and maintained as Terse RDF Triple Language (Turtle)[38] files in the iSamples Github[39], and published with the Australian Research Data Commons vocabulary service[40] or the ESIPFed Community Ontology Repository[41]. URIs are defined for each category and resolved using the W3ID re-direction service for Web applications[42]. We have opted to generate the URI tokens based on the preferred labels for the concepts, favoring user-friendliness over other considerations. Formal versioning policies for individual categories or the vocabulary as a unit have not been defined.

[33] https://isamplesorg.github.io/models/
[34] https://vocabs.ardc.edu.au/search/#!/?activeTab=vocabularies&q=isamples
[35] https://www.w3.org/RDF/
[36] https://www.w3.org/TR/skos-reference/
[37] https://www.ietf.org/rfc/rfc3986.txt
[38] https://www.w3.org/TR/turtle/
[39] https://github.com/isamplesorg/vocabularies/tree/develop/vocabulary
[40] https://vocabs.ardc.edu.au/search/#!/?activeTab=vocabularies&pp=15&q=isamples
[41] http://cor.esipfed.org/ont#/so/isample
[42] https://github.com/perma-id/w3id.org#permanent-identifiers-for-the-web

## 4. Vocabulary extensions

The vocabularies described in the previous section define categories at a high level, intended to cover material samples collected in any domain of interest. As such, they do not provide the granularity of categorization users in particular science communities will expect. To satisfy these use cases we expect user communities to develop extension vocabularies that provide the necessary granularity. The high-level vocabularies defined here provide a logical framework and extension points for these domain-specific vocabularies to be developed with more granular sub classes rooted in iSample vocabulary concepts. This approach will promote the development of extension vocabularies with a consistent logical basis, facilitating interoperability.

For example, in the geoscience community, classification of a sample as simply 'mineral' is too broad for most searches. A more specific mineral material classification is needed. As an example, we have implemented an extension vocabulary using the Nikel-Strunz mineral classification[43], which divides the domain of known minerals (with approximately 5800 species) into 10 classes[44] (Figure 7). This mineral group vocabulary has the iSample material 'mineral' as top concept, with the Nikel-Strunz classes as the child concepts in the vocabulary.

Other extension vocabularies might provide more granular subclasses under multiple concepts in the parent vocabulary. For instance in the materials extension for archaeological samples[45], various material

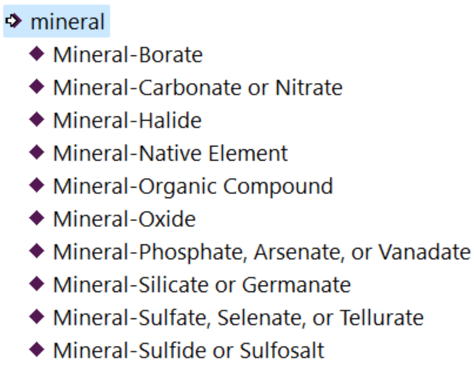


Fig. 6. Extension vocabulary for mineral groups. 'mineral' is a category in the iSamples material type vocabulary. It is the top concept in the extension vocabulary for more granular categorization of minerals.

[43] https://en.wikipedia.org/wiki/Nickel–Strunz_classification
[44] https://w3id.org/isample/earthenv/mingroup/1.0/mineralgroupvocabulary

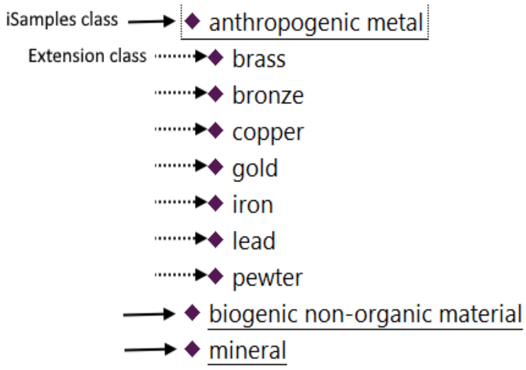


Fig. 8. Extract from material type extension vocabulary for archaeological materials. In this example, there are multiple top concepts in the extension vocabulary (the 'iSamples classes') that are categories in the base iSamples material type vocabulary. The extension vocabulary ('Extension classes') has more granular material type categories that are subtypes of the base categories. Subtypes for biogenic non-organic material and mineral are not shown in this figure.

types in the base iSamples vocabulary have more granular material type subclasses (Figure 8).

## 5. Implementation

The conceptual model for sample description was constructed first as a UML model[46]. The conceptual model is broadly based on the Sensor, Observation, Sample, and Actuator (SOSA) ontology [5] and the W3C Prov-O ontology [6]. The iSamples model adds some classes extending those models. The broad framework of the model is shown in the diagram in Figure 9. SamplingEvent has a related SamplingSite that accounts for the spatial context that was sampled. A material sample (sosa:Sample) has related curation activities that document processing and preservation of the sample after it has been collected. The sample is linked to an open world of other resources through the SampleRelation class, which implements the Digital Extended Specimen information graph [3]. Responsibility is a class linked to any prov:Activity subclass to document prov:Agent subclasses related to the activity through some role. IdentifierObject binds an identifier string with an authority agent that assures uniqueness of identifiers within some scope; any element that might be reused or referenced from an external source has an identifier. The model elements

[45] https://w3id.org/isample/opencontext/specimentype/0.1/oc_spectypevocab
[46] https://github.com/isamplesorg/metadata/blob/main/FullUMLModel.png

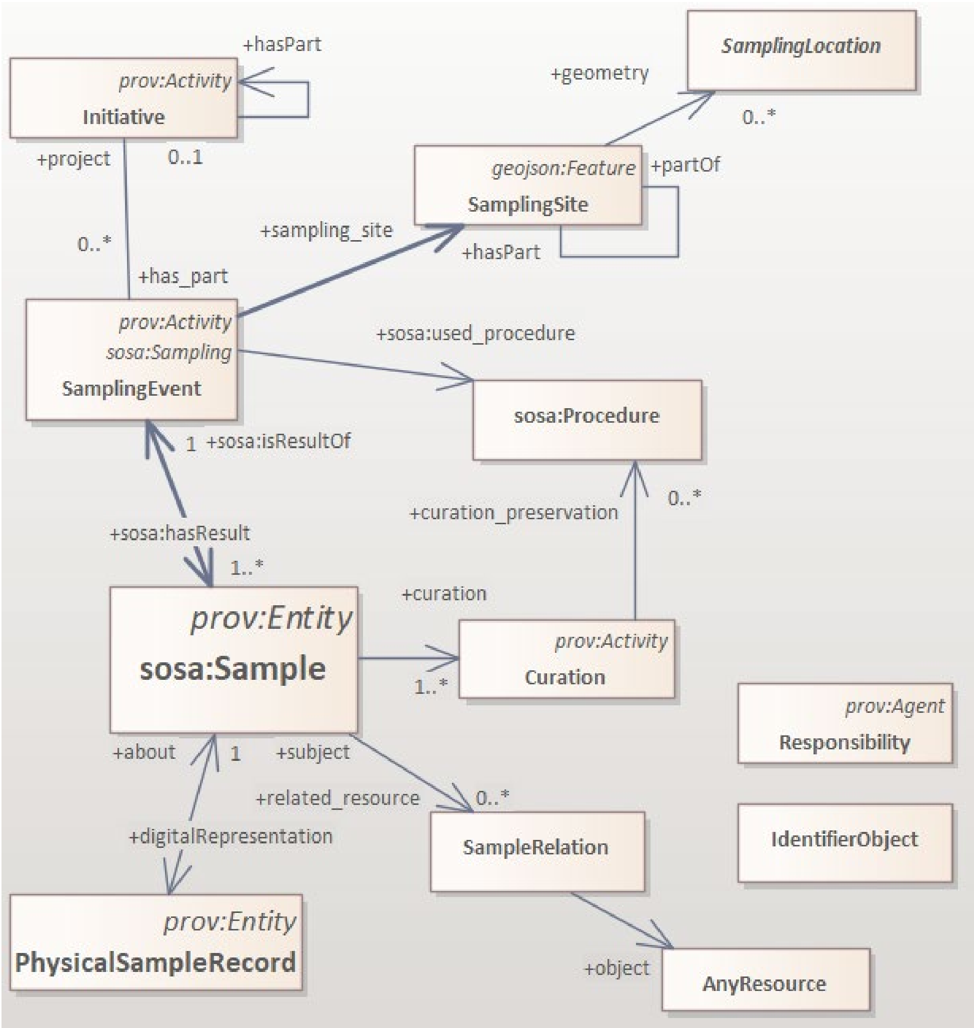


Fig. 9. Conceptual framework for material sample description. Class names in italics in the upper right of boxes are parent classes. Namespace abbreviations: prov- https://www.w3.org/TR/prov-o/, geojson – https://purl.org/geojson/vocab#, sosa: https://www.w3.org/ns/sosa/.

and properties are documented more fully on the iSamples web site[47]. The digital representation of the sample is a MaterialSampleRecord (a Digital Object), which is expected to include elements documenting all of the classes associated with the material sample.

The iSamples cyberinfrastructure uses the JSON format for serializing sample descriptions for information interchange between iSamples instances. The conceptual model is implemented using LinkML tools[48]. The entity and property schema is described using a simple key-value structure encoded with YAML[49] syntax. This schema definition file includes documentation for each entity and property[50]. The LinkML tools generate the JSON schema that can be used to validate metadata instances, as well as generating HTML web pages with documentation for the schema[51]. For version one, implementation focus has been on simplicity and compatibility with legacy sample descriptions. The use of complex property values has been minimized, favoring free text content.

[47] https://isamplesorg.github.io/metadata/
[48] https://linkml.io/linkml/
[49] https://yaml.org/spec/1.2.2/
[50] https://github.com/isamplesorg/metadata/blob/main/src/schemas/isamples_core.yaml
[51] https://isamplesorg.github.io/metadata/

Semantic interoperability is supported using URIs for responsible parties, iSamples controlled vocabulary terms, and optionally for keywords, as well as identifiers for SamplingEvents, SamplingSites, and Curation events. Properties that have text data type values can be populated with URIs, but the current user interface and search indexing will not take advantage of the linkages. Examples sample description instances can be found in the iSamples Github[52].

## 6. Relationships to other schemes and metadata formats

### *6.1. Schema.org*

A proposed mapping of the iSamples metadata scheme to schema.org properties is presented in a supplemental document in the iSamples Github[53], along with a proposed serialization of the iSamples metadata content using the Schema.org vocabulary [54]. Schema.org does not have properties that map to the iSamples sample curation property, or to the 'authorized_by' property related to permitting for a sampling event. Inclusion of this information can be done using the iSamples property URI as the key in the schema.org JSON. Schema.org is not designed for describing material samples, so usage of some properties does not follow the 'expected' domain or range for an entity-property pair. These interpretations of property semantics do not result in schema.org validation errors [55] because of the loose 'domainIncludes' and 'rangeIncludes' predicates used in the schema.org RDF schema[56], but various warnings are raised by the validator, flagging the unexpected usages. This is a work in progress.

### *6.2. IGSN and DataCite*

The International Generic Sample Number (IGSN) sample registration system has been migrated to use digital object identifiers (DOIs) managed by DataCite. Thus, all IGSN sample metadata will be serialized using the DataCite metadata schema. A DataCite workgroup has developed recommendations for serializing material sample descriptions using the DataCite metadata schema[57]. Mappings from the original IGSN registration and description metadata scheme and from the DataCite v4.3 XML metadata schema to the iSamples JSON implementation are documented in the iSamples GitHub[58]. Note that there are some minor discrepancies between the DataCite XML[59] and JSON[60] serialization. The XML schema appears to be more widely used, but the JSON schema offers some useful open-world flexibility.

### *6.3. TDWG Minimum Information about a Digital Specimen (MIDS)*

Minimum Information about a Digital Specimen (MIDS)[61] is a specification defining information elements expected in a digital representation of a 'physical specimen', interpreted here to be equivalent to iSamples 'material sample'. The MIDS specification defines four levels of content for sample description, level 0 to level 3. The scope is focused on curated natural science collections (typically in museums), with the goal of making descriptions of physical objects available on the World Wide Web. Higher content levels include more detail in the sample description. This digital specimen object corresponds to the iSamples sample description record. A mapping from the MIDS digital specimen, levels 0-3 (including some yet-to-be adopted properties) is included in the iSamples Github[62].

### *6.4. Digital extended specimen*

The Digital extended specimen (DES) is a web-accessible representation of the digital assets related to a material sample (physical specimen) [3]. These assets can include observations and measurements from the specimen, its sample context (sampled feature), or analyzed derivatives from an original material sample. This concept has evolved into the Open Digital Specimen (OpenDS) as the basis for the Distributed System

[52] https://github.com/isamplesorg/metadata/tree/main/examples
[53] https://github.com/isamplesorg/metadata/blob/main/schemaMapping/schema.org-iSamplesMapping.csv
[54] https://github.com/isamplesorg/metadata/tree/main/notes/schemaOrg
[55] See https://validator.schema.org/
[56] https://schema.org/version/latest/schemaorg-current-https.jsonld
[57] https://support.datacite.org/docs/igsn-id-metadata-recommendations
[58] https://github.com/isamplesorg/metadata/tree/main/schemaMapping
[59] https://github.com/datacite/schema/blob/master/source/meta/kernel-4.3/metadata.xsd
[60] https://github.com/datacite/schema/blob/master/source/json/kernel-4.3/datacite_4.3_schema.json
[61] https://github.com/tdwg/mids/blob/working-draft/current-draft%20/MIDS-definition-v0.17-13Jul2023.md
[62] https://github.com/isamplesorg/metadata/blob/main/schemaMapping/MIDS-iSamplesMapping.csv

of Scientific Collections (DiSSCo)[63] activity in the pan-European Research Infrastructure. The DiSSCo vision is a seamless and standardized digital representation of material samples in Natural Science Collections. While the DiSSCo vision parallels the goals of the iSamples project, it is founded in the Global Biodiversity Community, presenting opportunities for harmonization and interoperability of these efforts to enable integration of samples across these domains. The OpenDS metadata schema[64] incorporates elements from Darwin Core, with numerous extensions specific to material samples. A mapping from iSamples JSON metadata to the OpenDS metadata schema is included in the iSamples Github[65].

## 7. Testing

The mapping from the iSamples material sample description scheme to other similar schemes described in the last section demonstrates the utility of the iSamples scheme as a data integration format. The JSON schema for iSamples material sample description has been tested in greater depth via the process of mapping content from partner systems into the iSamples central aggregator[66]. Some minor issues have emerged, leading to updates in the core vocabulary or the metadata schema. The version 1 release tags are intended to provide a stable snapshot that other parties can use to implement a sample description and registration that can be integrated with the iSamples infrastructure or used for cross-domain sample description applications.

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[64] https://github.com/DiSSCo/openDS/blob/master/data-model/digitalobjects/0.1.0/digital-specimens/schema/digital-specimen.json

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