

FIAS REGISTRY OF RESEARCH SPECIFICATIONS

Minimal Acquisition Manifest for Synchrotron Spectral Maps of Ancient Materials

REGISTRY IDENTIFIER

FOAR-CON2X-HTWHZ4W97

VERSION

0.9

OBJECT TYPE

Data model or interchange format

SUBJECT AREA

Chemistry and materials science

DOCUMENT MATURITY

Candidate for stable use

SUBMITTED

17 June 2014, 12:00 UTC

PUBLISHED

03 October 2014, 12:00 UTC

LICENCE

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AUTHORITATIVE VERSION

Registration records the outcome of the Registry review for this version: the submission was sufficiently identified, documented, and internally determinate for the stated procedure. Scope, adoption, and competing conventions are documented separately where relevant.

REGISTRY STATUS**Accepted for registration**

03 October 2014, 12:00 UTC

Core description

SUBMISSION KIND

New registry concept

FULL TITLE

Minimal Acquisition Manifest for Synchrotron Spectral Maps of Ancient Materials

SHORT TITLE OR ACRONYM

MASM-AM

OBJECT TYPE

Data model or interchange format

STATUS CLAIMED BY THE SUBMITTER

Experimental specification

MATURITY OF THIS VERSION

Candidate for stable use

VERSION

0.9

PRINCIPAL SUBJECT AREA

Chemistry and materials science

KEYWORDS

- heritage science
- synchrotron spectroscopy
- spectral imaging
- acquisition metadata
- ancient materials

PROBLEM, SCOPE, AND EXCLUSIONS

Multimodal maps of archaeological and heritage samples can become impossible to reinterpret when spatial calibration, beam energy, detector geometry or sample orientation is detached from the intensity array. This profile prescribes a small sidecar manifest for two- and three-dimensional synchrotron spectral maps. Its scope is acquisition and calibration metadata; chemical interpretation, attribution, conservation treatment and legal ownership of the object require separate records.

INTENDED USERS AND CONTEXTS

- Scientists acquiring X-ray, UV-visible or infrared spectral maps of ancient materials
- Data curators receiving maps from synchrotron experiments
- Conservators evaluating whether an archived dataset can be reanalysed

RELATION TO EXISTING PRACTICE

Codifies an existing practice

SCIENTIFIC CONTEXT, SOURCES, AND SCHOLARLY DISCUSSION

This section describes the scientific background, underlying work, and sources of the specification, together with the research groups and scholarly settings in which the proposed solution or its formalisation was presented or discussed. It documents the context and nature of these scholarly exchanges.

Synchrotron studies of archaeological and historical materials combine measurements at different spatial scales and with different spectroscopic and imaging methods. L. Bertrand et al. (2011, 2012) describe this research programme through the IPANEMA platform at SOLEIL and its applications to cultural-heritage materials. The interpretation of a spectral map depends on its experimental context: beam energy, detector geometry, spatial calibration, sample orientation and the relation between coordinates and intensity arrays.

IPANEMA brings together the analytical questions of heritage research and the methods of synchrotron measurement, including work by L. Bertrand, L. Robinet, M. Thoury and S. X. Cohen. The exchange of results between these fields requires acquisition information that remains understandable after a dataset leaves the instrument environment. This need motivates a compact record linking a sample to one two- or three-dimensional spectral map.

The profile expresses that record as a JSON manifest accompanying HDF5, EDF or TIFF data. It records axes, units, calibration and provenance in a form that can be checked against the associated arrays and files. JSON Schema Draft 4 supplies a machine-readable basis for validating the manifest. Retaining these relationships allows another researcher to locate the measured region, interpret the coordinate system and recover the conditions under which the map was acquired.

References:

- Bertrand L. et al. European research platform IPANEMA at the SOLEIL synchrotron for ancient and historical materials. J Synchrotron Radiat. 2011;18:765–772. DOI: <https://doi.org/10.1107/S090904951102334X>
- Bertrand L. et al. Cultural heritage and archaeology materials studied by synchrotron spectroscopy and imaging. Appl Phys A. 2012;106:377–396. DOI: <https://doi.org/10.1007/s00339-011-6686-4>
- Bertrand L., Thoury M., Anheim E. Ancient materials specificities for their synchrotron examination and insights into their epistemological implications. Journal of Cultural

Heritage. 2013;14(4):277–289; published July 2013. DOI: <https://doi.org/10.1016/j.culher.2012.09.003> ; Author bibliography: <https://cv.hal.science/mathieu-thoury>
- JSON Schema, Core definitions and terminology, Draft 4, 2013. Source: <https://json-schema.org/draft-04/json-schema-core>

EXTERNAL STANDARDISATION STATUS

None intended

LICENCE FOR THE SUBMITTED SPECIFICATION

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PUBLICATION DECLARATION

Yes

Data model or interchange format

ENTITIES, RECORDS, AND RELATIONSHIPS

Study contains one or more Samples. Sample has one or more Acquisitions. Acquisition references a DataArray, Detector, SpatialAxis, SpectralAxis and at least one Calibration. A Provenance event records the facility, beamline, operator role and acquisition time. Interpretations may reference an acquisition and remain outside the normative manifest.

SERIALIZATION AND MEDIA TYPE

UTF-8 JSON, media type application/json. The manifest is stored beside, and refers by relative URI and SHA-256 digest to, an unchanged facility-native data file.

REQUIRED FIELDS AND CARDINALITIES

Root: profile_version exactly one; study_id exactly one; samples one or more. Sample: local_sample_id, material_description, orientation_note. Acquisition: acquisition_id, start_time, facility, beamline, technique, data_file, sha256, detector, two or three spatial_axes, spectral_axis and calibrations. Each axis requires label, unit, length and calibration expression or lookup URI.

DATATYPES, CONTROLLED VALUES, NULLS, AND UNKNOWN VALUES

Identifiers are non-empty strings; timestamps use RFC 3339 with offset; units use UCUM strings where available; axis lengths are positive integers; numeric values are JSON numbers. Unknown values are represented by an explicit null accompanied by an `unknown\_reason`; absent and unknown have distinct meanings.

MACHINE VALIDATION MECHANISM

JSON Schema

VALIDATOR, SCHEMA, OR GRAMMAR DETAILS

A Draft-04 JSON Schema validates cardinalities, timestamps, SHA-256 syntax, positive dimensions and the controlled technique list. Physical correctness of calibration is checked by the conformance test.

FORWARD AND BACKWARD COMPATIBILITY

Patch releases may add optional properties only. Readers preserve unknown optional properties and reject a different major version. Facility data remain byte-identical, preserving compatibility with NeXus/HDF5/EDF/TIFF readers.

COMPLETE MINIMAL EXAMPLE

```
{  
  "profile_version": "0.9",
```

```
"study_id": "ipanema-example-17",
"samples": [{
  "local_sample_id": "S17",
  "material_description": "paint microsample",
  "orientation_note": "surface normal toward beam",
  "acquisitions": [{
    "acquisition_id": "A17-XRF",
    "start_time": "2014-05-12T09:14:00+02:00",
    "facility": "SOLEIL",
    "beamline": "example",
    "technique": "XRF-map",
    "data_file": "A17.edf",
    "sha256":
"0000000000000000000000000000000000000000000000000000000000000000",
    "detector": {"model": "recorded-in-lab-book"},
    "spatial_axes": [
      {"label": "x", "unit": "um", "length": 128, "calibration": "x=i*2"},
      {"label": "y", "unit": "um", "length": 64, "calibration": "y=j*2"}
    ],
    "spectral_axis": {"label": "energy", "unit": "keV", "length":
2048, "calibration": "lookup:energy.csv"},
    "calibrations": [{"type": "energy", "reference": "energy.csv"}]
  }]
}]
}
```

Registry review record

Submission received

17 June 2014, 12:00 UTC

Submission received.

Accepted for registration

03 October 2014, 12:00 UTC

Accepted as a narrow archival sidecar profile for reproducible acquisition context. Broader heritage-science formats require separate review; the conformance test must include digest, dimension and calibration checks.