Formalisation of materials characterisation terminology and application to industrial protocols

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NanoMECommons Open Day

Cambridge, 20 November 2024

Goal

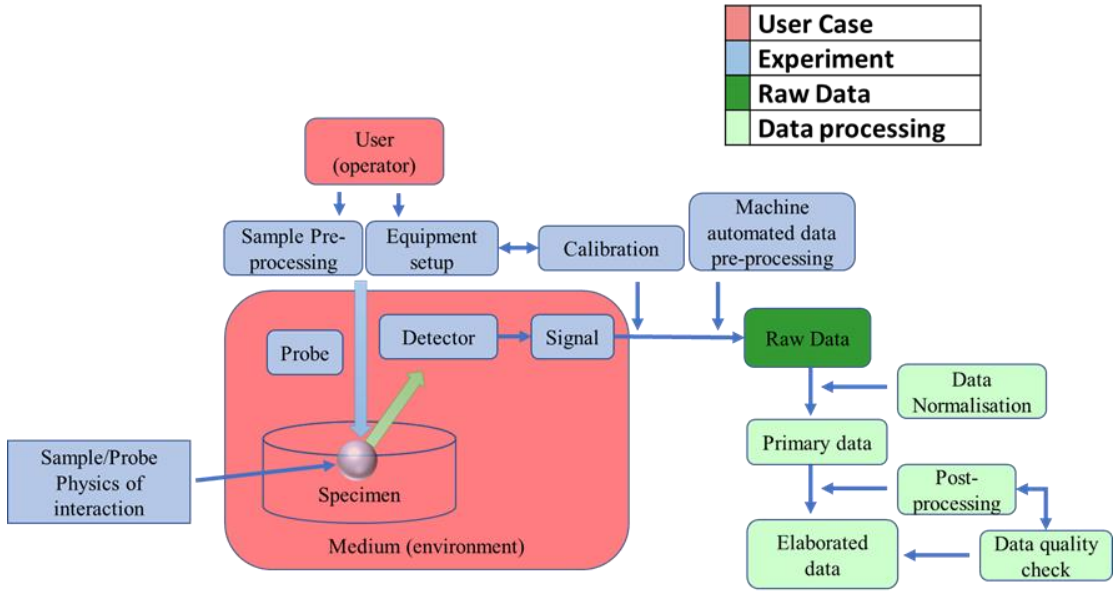
- A framework for a clear semantic and diagrammatic representation of characterisation experiments and protocols
- Human and machine readable
- Facilitates
  - Interoperability between systems
  - Communication between operators
  - Search and retrieve

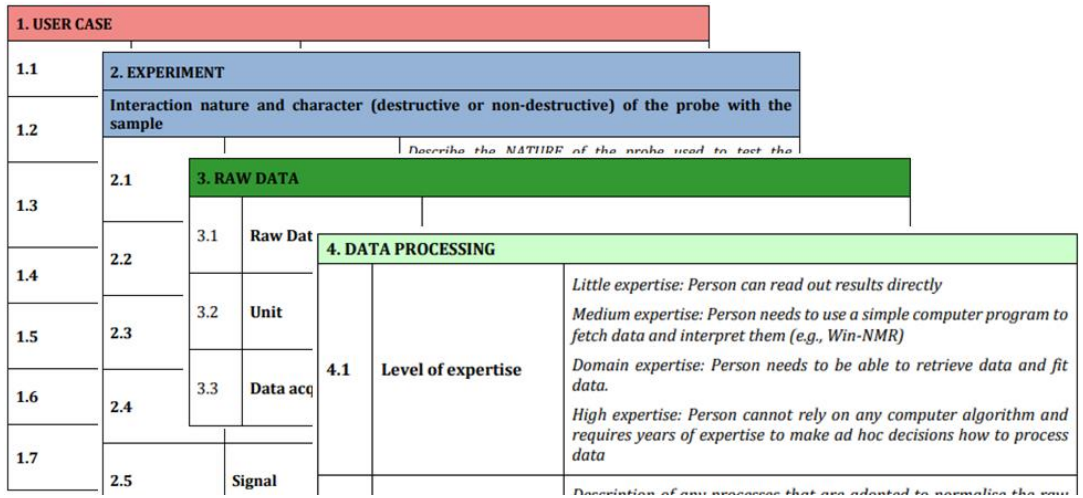
The starting point: CHADA

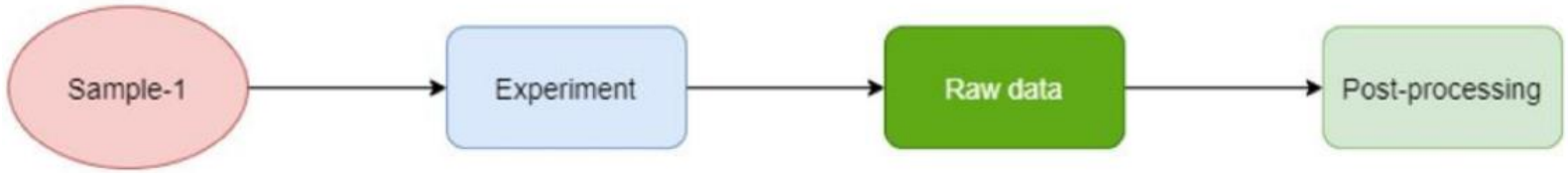
A common language and formal approach how to log a characterisation project

CWA 17815 "Materials characterisation - Terminology, metadata and classification "
https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf

New CWA ongoing

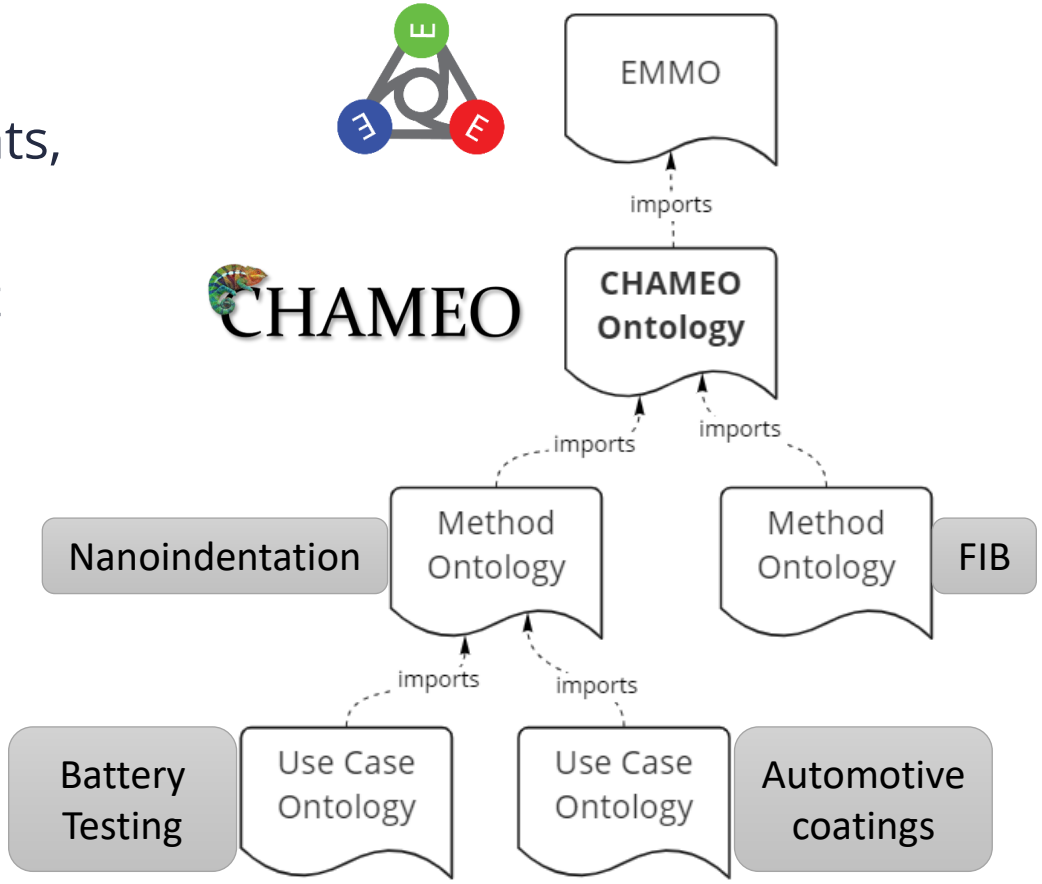






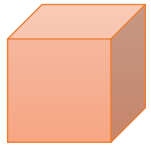
CHAMEO (CHaracterisation MEthodology Ontology)

- CHAMEO: a framework for defining a clear, machine-readable documentation of characterisation experiments, based on shared concepts and definitions
- The CHAMEO ontology models the generic aspects that are in common across the different characterisation techniques
- Specific ontologies, modelling the different characterisation techniques, can be developed by specialising the CHAMEO definitions
- This follows a modular design approach that increases the level of reusability and interoperability

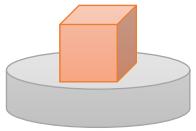


The CHAMEO ontology development is supported by an EMMC Task Group.

What is in CHAMEO?



Material/Batch



Sample

- Dimensions
- Structure (e.g. layers)
- Material's physical and chemical composition
- Hazard

Characterisation procedures

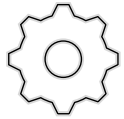
Sample extraction	Sample preparation	Sample inspection
Calibration process	Measurement system adjustment	Characterisation measurement process
Data preparation	Data post-processing	Data validation

Characterisation Data

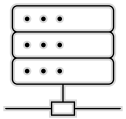
- Calibration data
- Raw data
- Primary data
- Secondary data
- Characterisation property

Operator

Laboratory



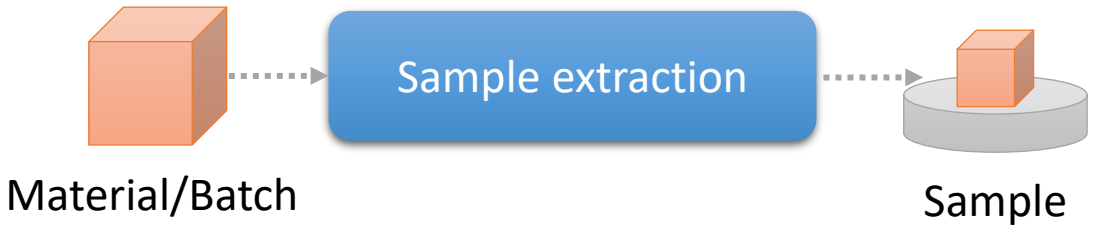
Instrument

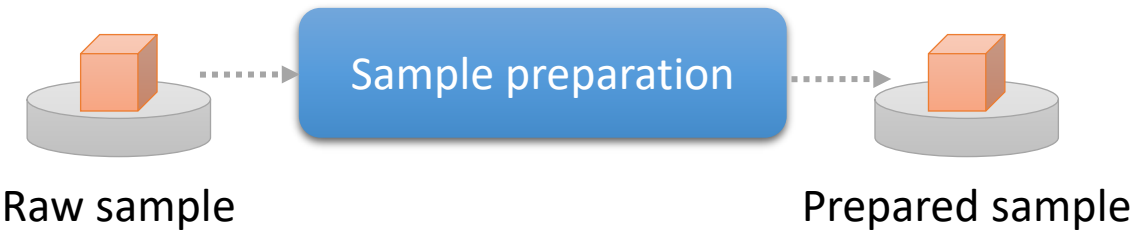


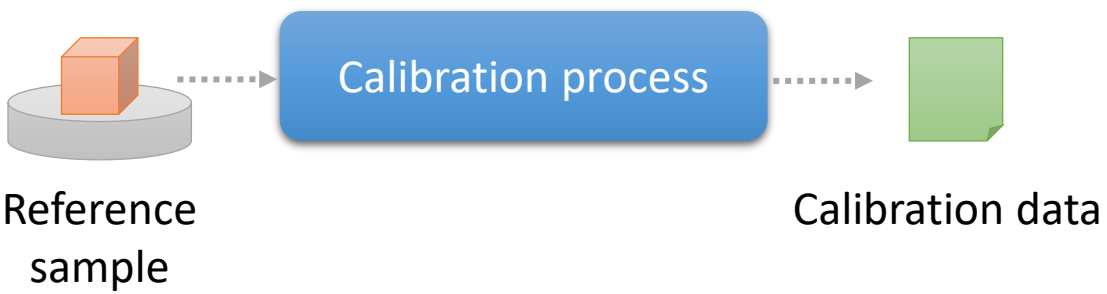
Environment, Parameters

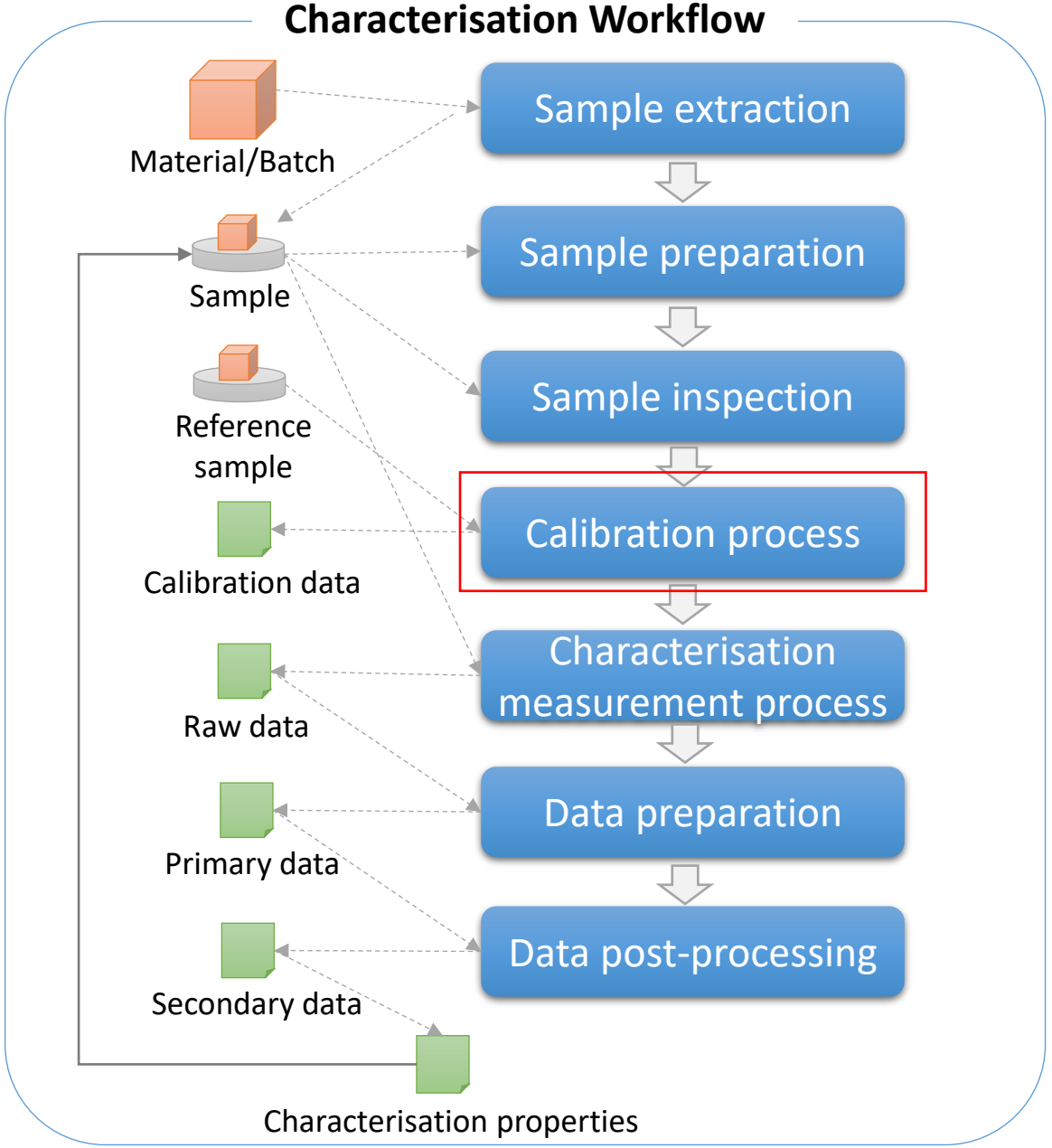
Level of expertise

CHAMEO is flexible!

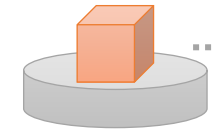








The characterisation process can be break-down to the desired level of details



Fused silica

Nanoindentation calibration process (workflow)

Microscope to indenter calibration → Tip area function → Compliance calibration → Continuous Stiffness Measurement

Calibration data

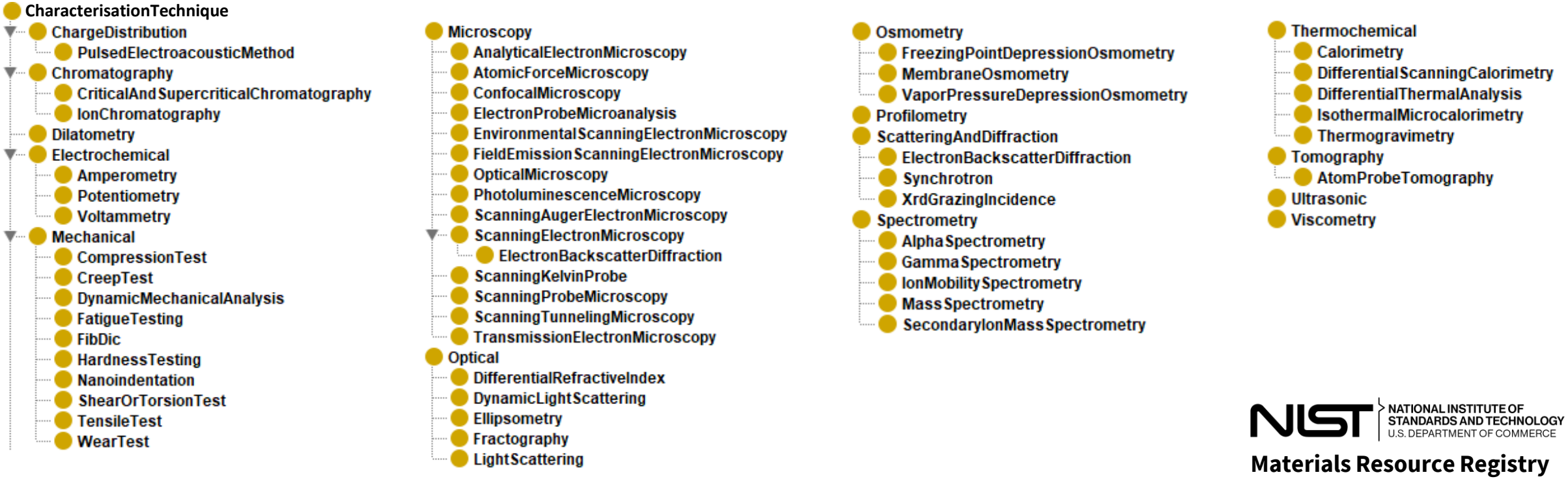
- Load
- Displacement
- Drift rate

Continuous Stiffness Measurement (workflow)

Surface detection and thermal drift stabilization → Moving to actual test locations → Surface approach and detection → Dynamic loading to Target Load/Target depth and final unloading.

Taxonomy of Characterisation Techniques

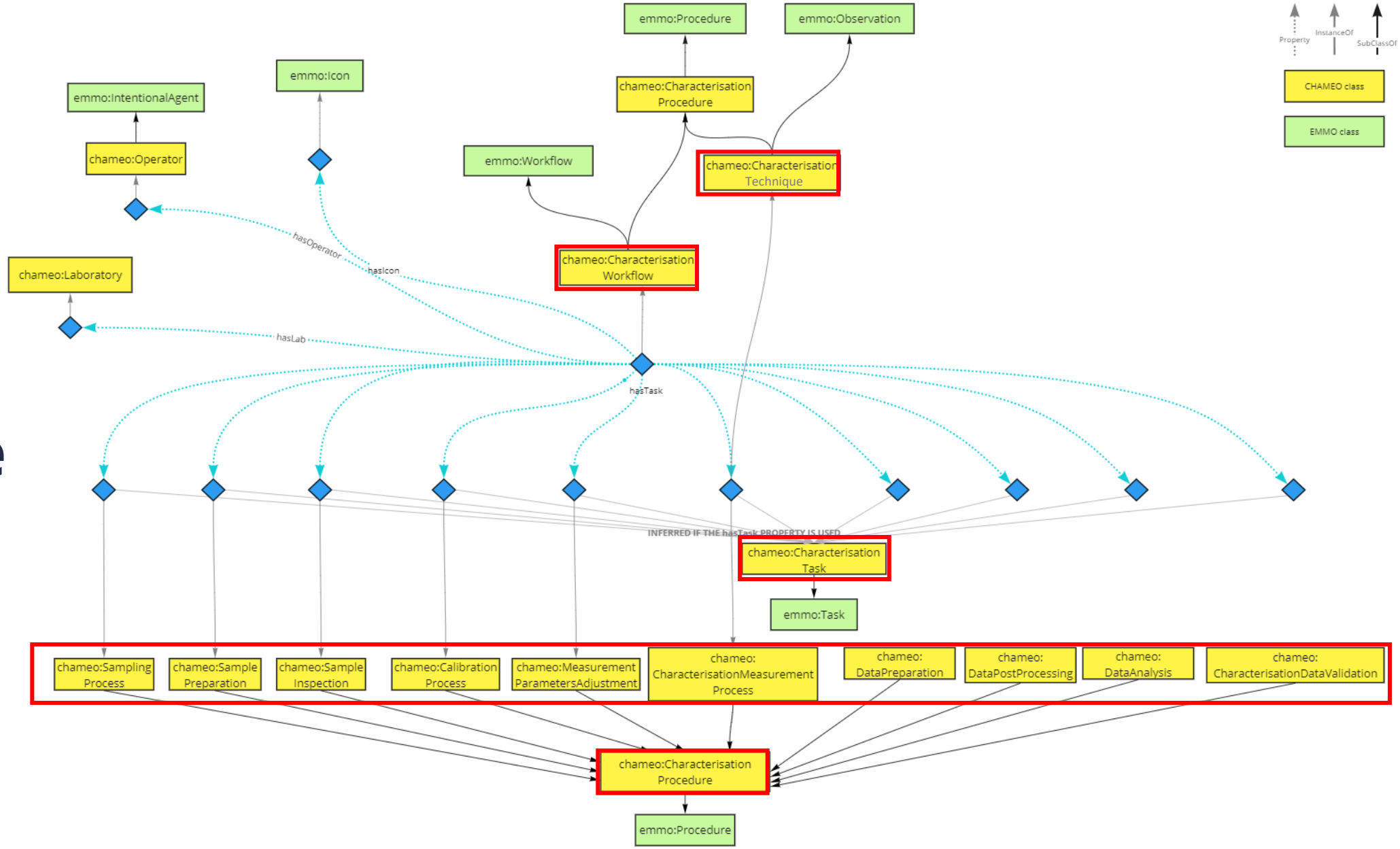
- Introduction of a taxonomy for the characterisation techniques, based on a de-facto standard (NIST, RDA)



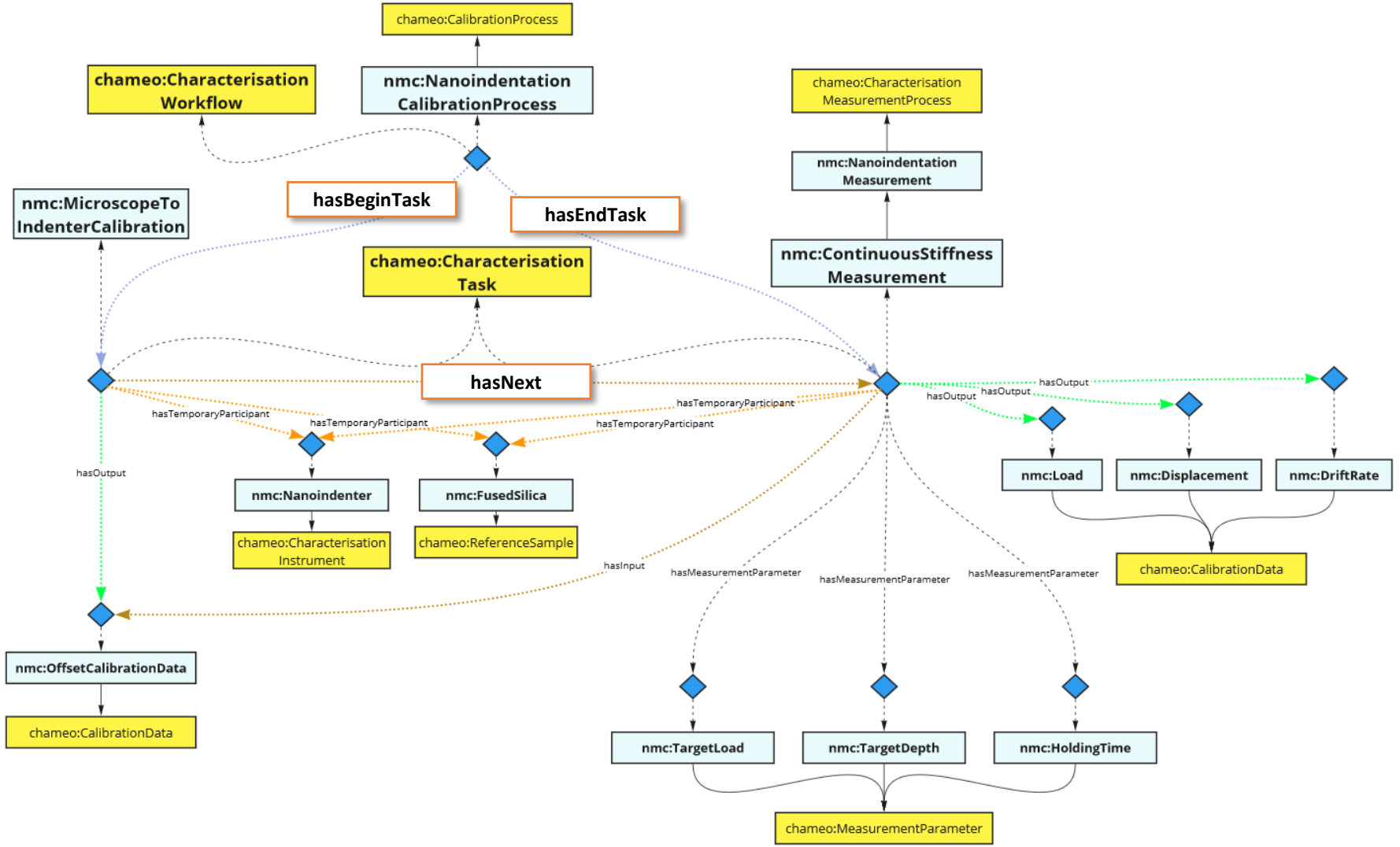
NIST NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY U.S. DEPARTMENT OF COMMERCE

Materials Resource Registry

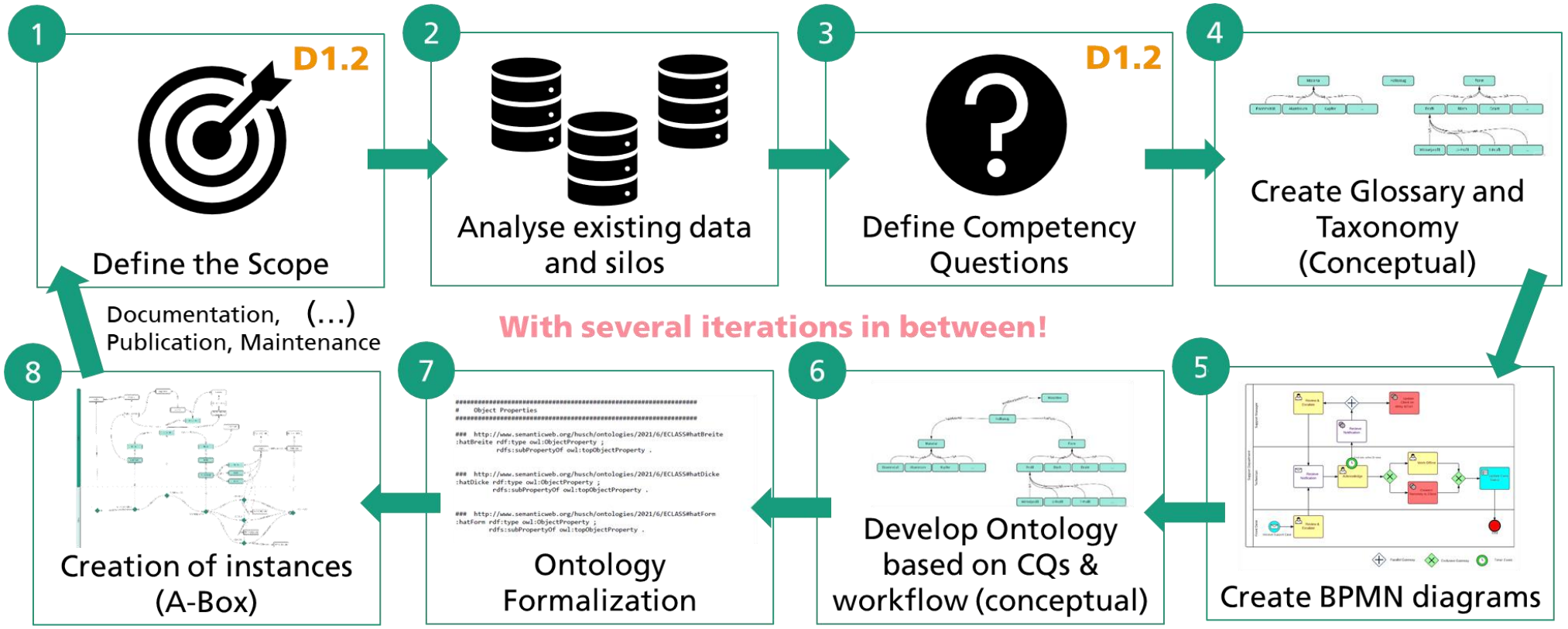
CHAMEO Structure



Simplified Nanoindentation calibration process represented as a workflow through the ontology



Ontology design process

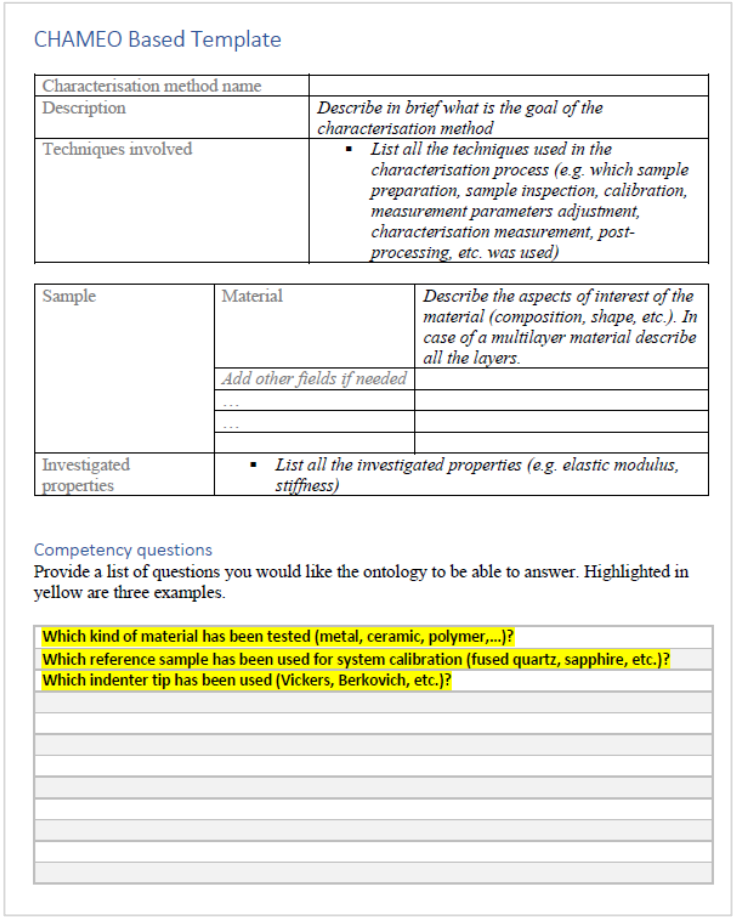


Web protégé
Collaborative environment

CAMUNDA

CHAMEO-based template

- To speed-up the collection of requirements for the development of the next ontologies
- Agreed to be used as a basis for the development of the new CHADA form during the ongoing CWA



CHAMEO Based Template

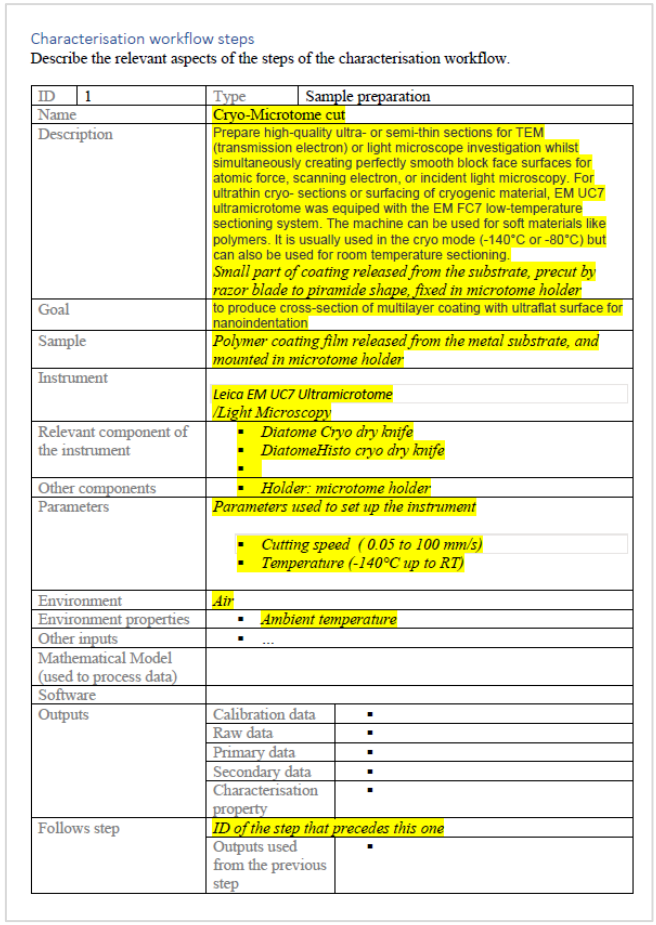
Characterisation method name	
Description	*Describe in brief what is the goal of the characterisation method*
Techniques involved	▪ *List all the techniques used in the characterisation process (e.g. which sample preparation, sample inspection, calibration, measurement parameters adjustment, characterisation measurement, post-processing, etc. was used)*

Sample	Material	*Describe the aspects of interest of the material (composition, shape, etc.). In case of a multilayer material describe all the layers.*
	Add other fields if needed	
	…	
	…	
Investigated properties	▪ *List all the investigated properties (e.g. elastic modulus, stiffness)*	

Competency questions

Provide a list of questions you would like the ontology to be able to answer. Highlighted in yellow are three examples.

Which kind of material has been tested (metal, ceramic, polymer,…)?
Which reference sample has been used for system calibration (fused quartz, sapphire, etc.)?
Which indenter tip has been used (Vickers, Berkovich, etc.)?



Characterisation workflow steps

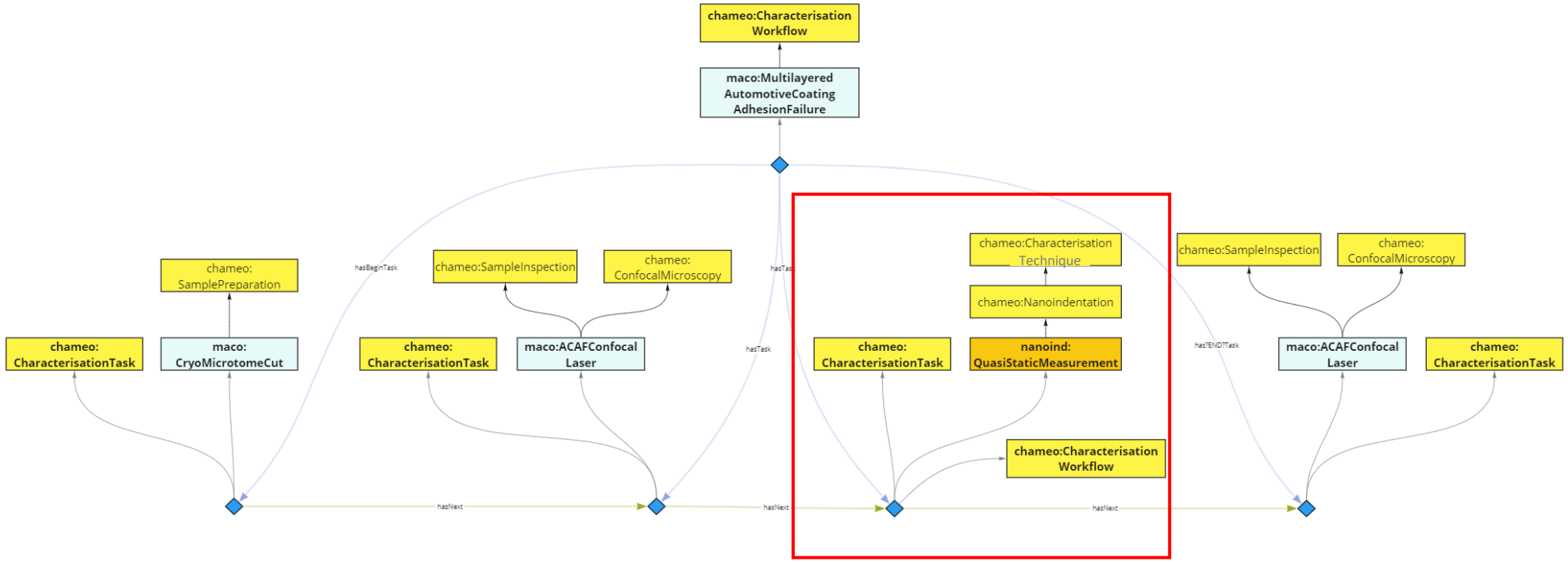
Describe the relevant aspects of the steps of the characterisation workflow.

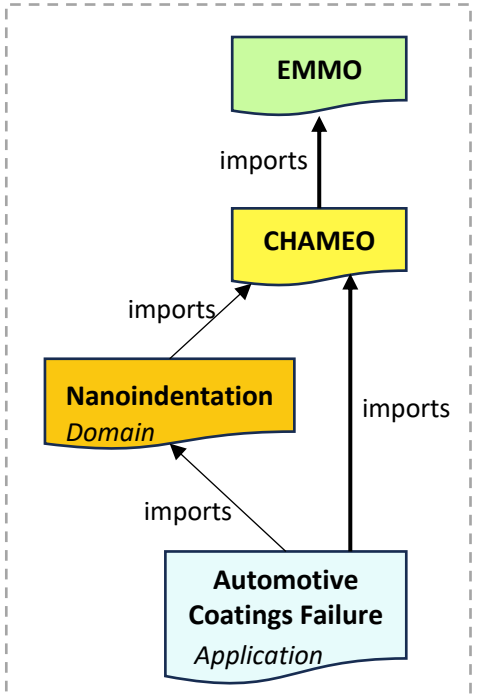
ID	1	Type	Sample preparation
Name		Cryo-Microtome cut	
Description		Prepare high-quality ultra- or semi-thin sections for TEM (transmission electron) or light microscope investigation whilst simultaneously creating perfectly smooth block face surfaces for atomic force, scanning electron, or incident light microscopy. For ultrathin cryo- sections or surfacing of cryogenic material, EM UC7 ultramicrotome was equiped with the EM FC7 low-temperature sectioning system. The machine can be used for soft materials like polymers. It is usually used in the cryo mode (-140°C or -80°C) but can also be used for room temperature sectioning. *Small part of coating released from the substrate, precut by razor blade to piramide shape, fixed in microtome holder*	
Goal		to produce cross-section of multilayer coating with ultraflat surface for nanoindentation	
Sample		*Polymer coating film released from the metal substrate, and mounted in microtome holder*	
Instrument		*Leica EM UC7 Ultramicrotome /Light Microscopy*	
Relevant component of the instrument		▪ *Diatome Cryo dry knife* ▪ *DiatomeHisto cryo dry knife* ▪	
Other components		▪ *Holder: microtome holder*	
Parameters		*Parameters used to set up the instrument* ▪ *Cutting speed (0.05 to 100 mm/s)* ▪ *Temperature (-140°C up to RT)*	
Environment		*Air*	
Environment properties		▪ *Ambient temperature*	
Other inputs		▪ …	
Mathematical Model (used to process data)			
Software			
Outputs	Calibration data	▪	
	Raw data	▪	
	Primary data	▪	
	Secondary data	▪	
	Characterisation property	▪	
Follows step		*ID of the step that precedes this one*	
	Outputs used from the previous step	▪	

Ontologies based on CHAMEO

- Technique specific
  - Nanoindentation testing
  - FIB-DIC
- Industrial use-cases
  - Automotive coatings – BASF
  - Advanced High-Strength Steels - CRF
  - Organic electronic devices - OET
  - Superhydrophobic nanopatterned surfaces – TRT
  - Battery testing – KEYS
    - Publication in *Computers in industry* https://doi.org/10.1016/j.compind.2024.104203

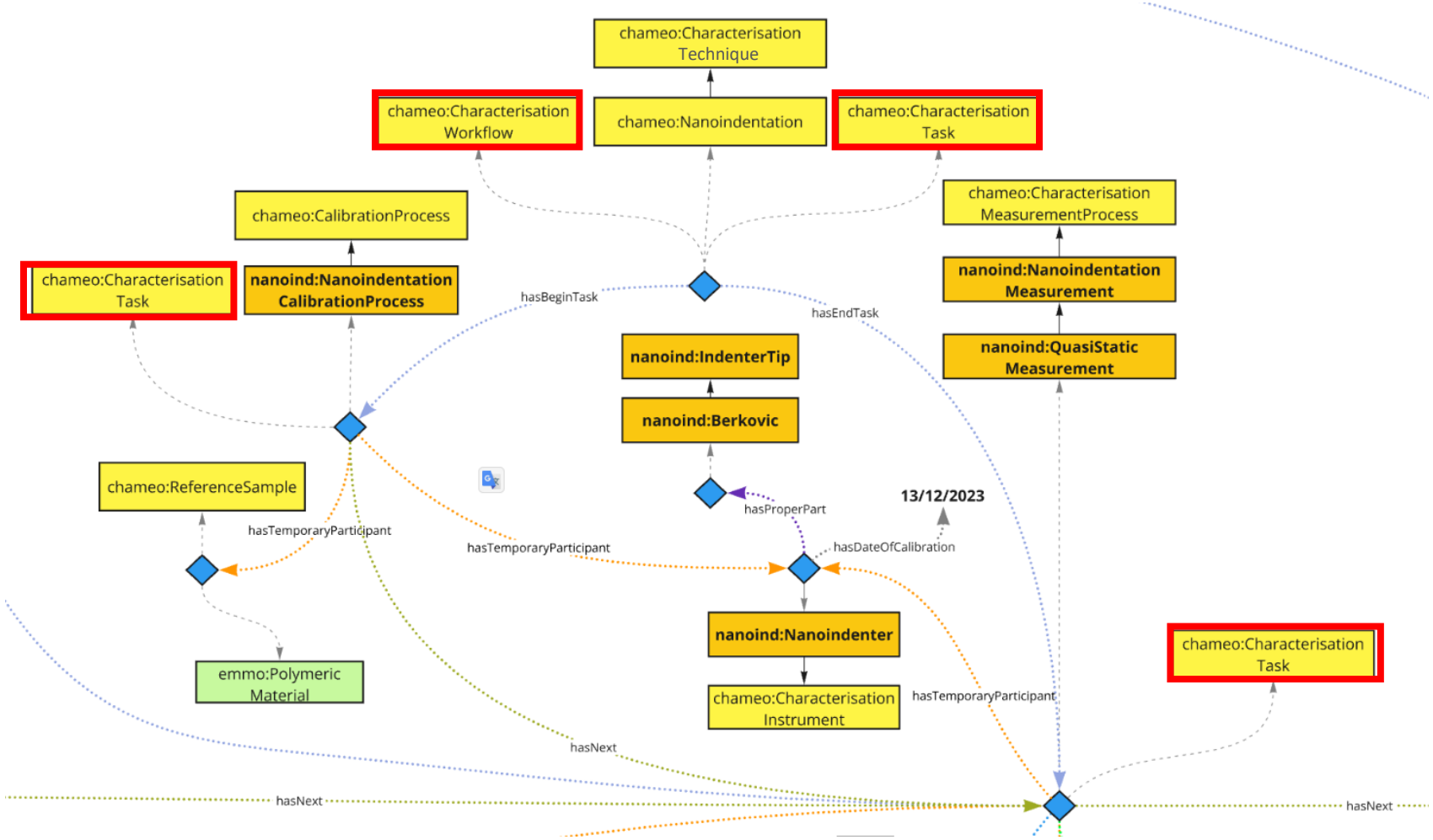
Multilayered Coatings Failure Testing
Industrial use-case from BASF





Multilayered Coatings Failure Testing
Industrial use-case from BASF

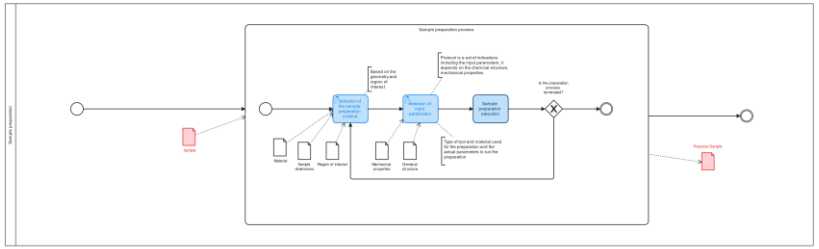
Nanoindentation is
a task of this workflow
but is itself a workflow
(here calibration + measurement)
that can be breakdown in details



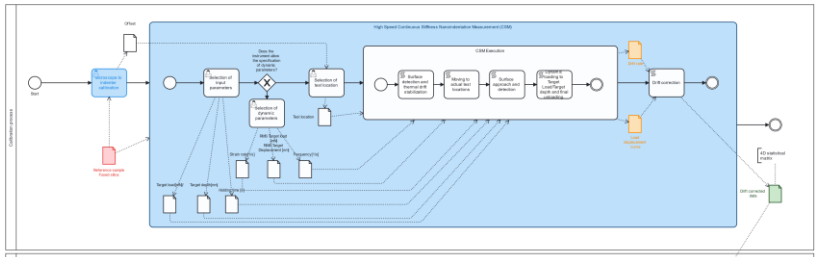
BPMN to diagrammatic represent Characteristion Workflows

Nanoindentation

SAMPLE PREPARATION
> *Decision process*

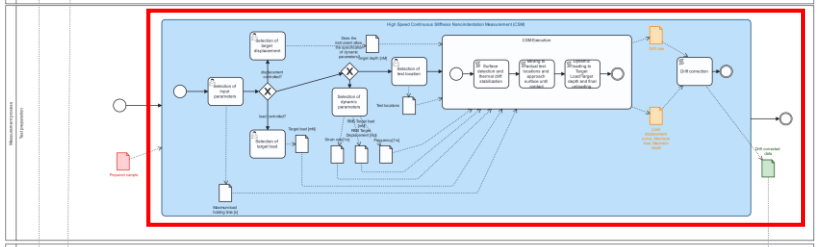


CALIBRATION

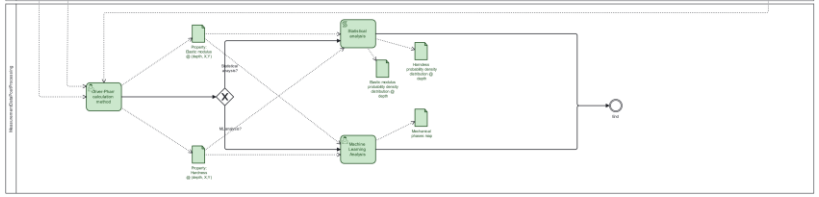


CALIBRATION DATA POST-PROCESSING

MEASUREMENT



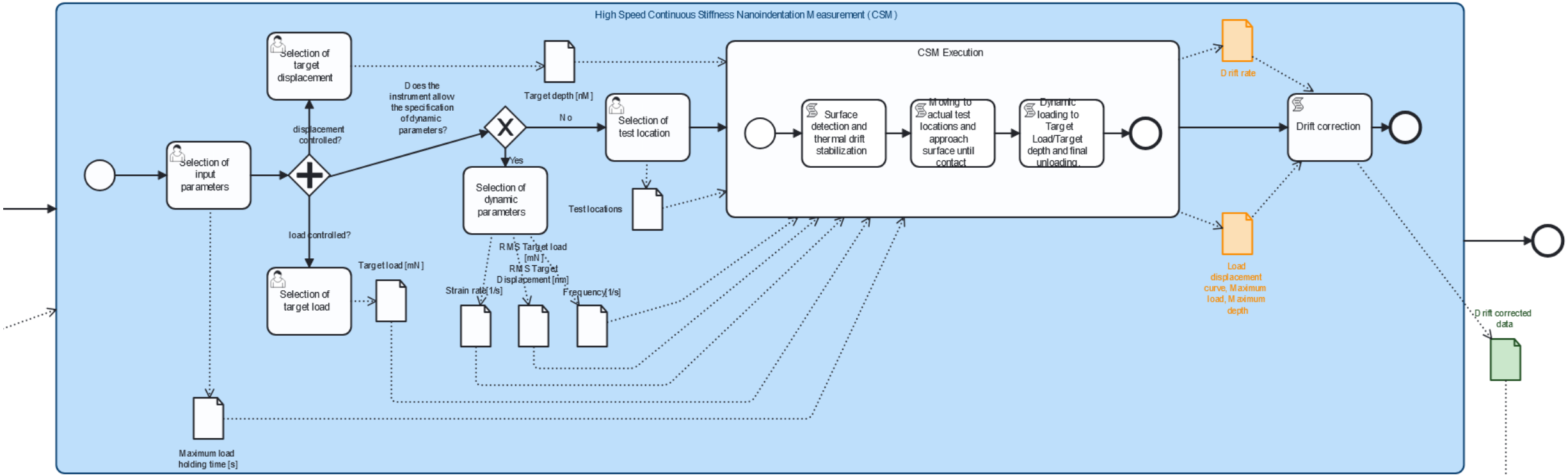
MEASUREMENT DATA POST-PROCESSING



LINK

Nanoindentation

SAMPLE PREPARATION
> Decision process



MEASUREMENT DATA POST-PROCESSING

LINK

BPMN to diagrammatic represent Characteristion Workflows

Multilayered Coatings industrial use-case (BASF)

SAMPLE PREPARATION
> *Cryotome cut*

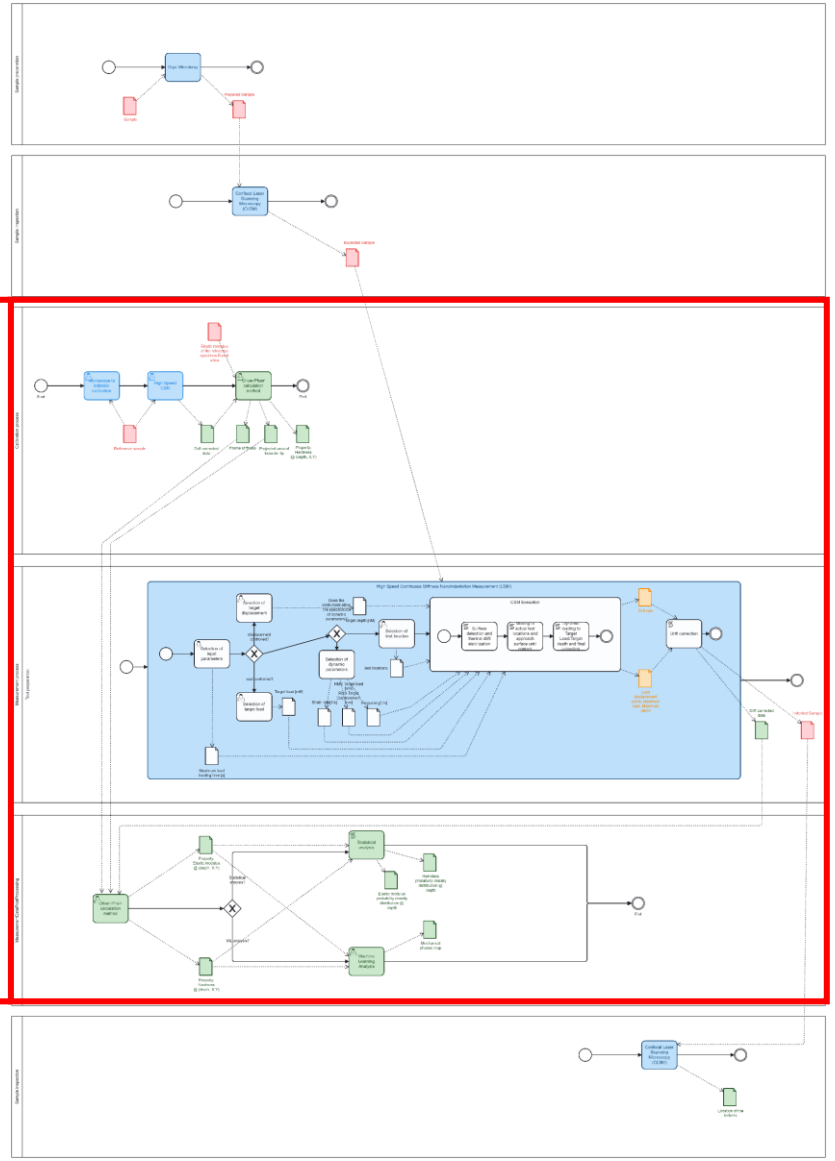
SAMPLE INSPECTION
> *CLSM*

CALIBRATION
> *Nanoindentation*

MEASUREMENT
> *Nanoindentation*

POST-PROCESSING
> *Nanoindentation*

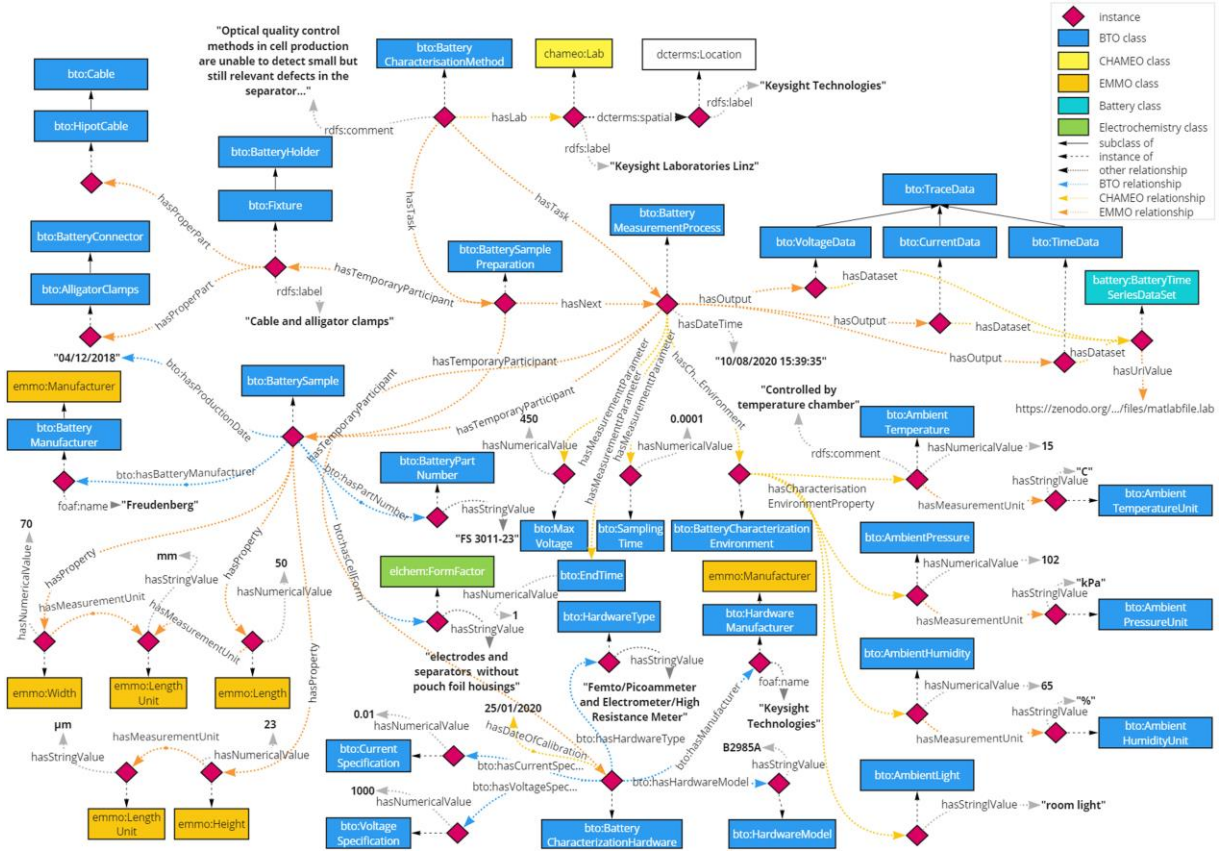
SAMPLE INSPECTION
> *CLSM*



LINK

Battery Testing
Industrial Use Case from Keysight

- Provide a unified and versatile structure for organising knowledge and data in battery testing and battery quality control.
- Models a range of electrical battery cell tests, including impedance spectroscopy, self-discharge, and high-voltage
- Ontology to support the design of a test experiment

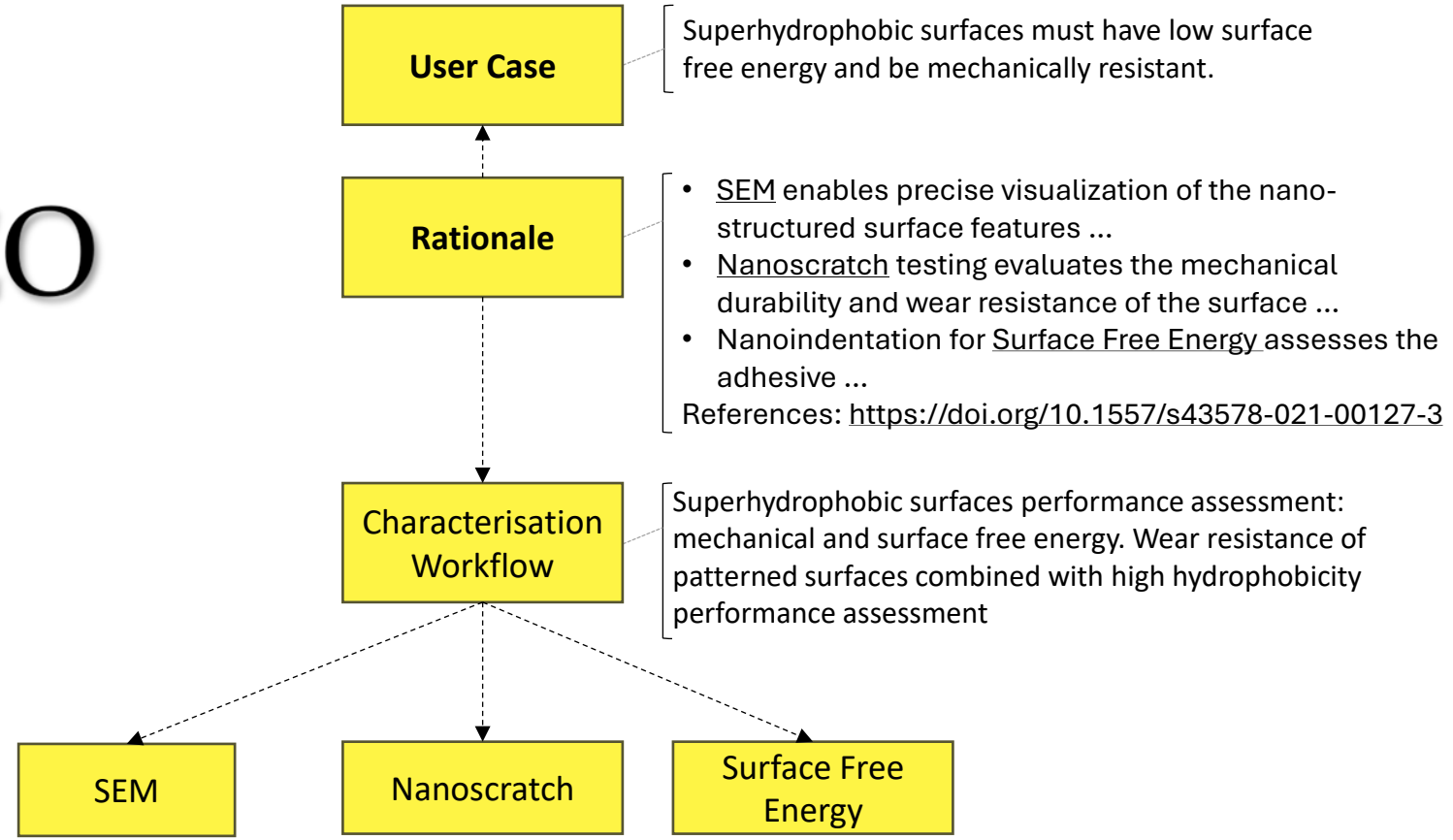


Battery testing ontology: An EMMO-based semantic framework for representing knowledge in battery testing and battery quality control
Computers in Industry, https://www.sciencedirect.com/science/article/pii/S0166361524001313

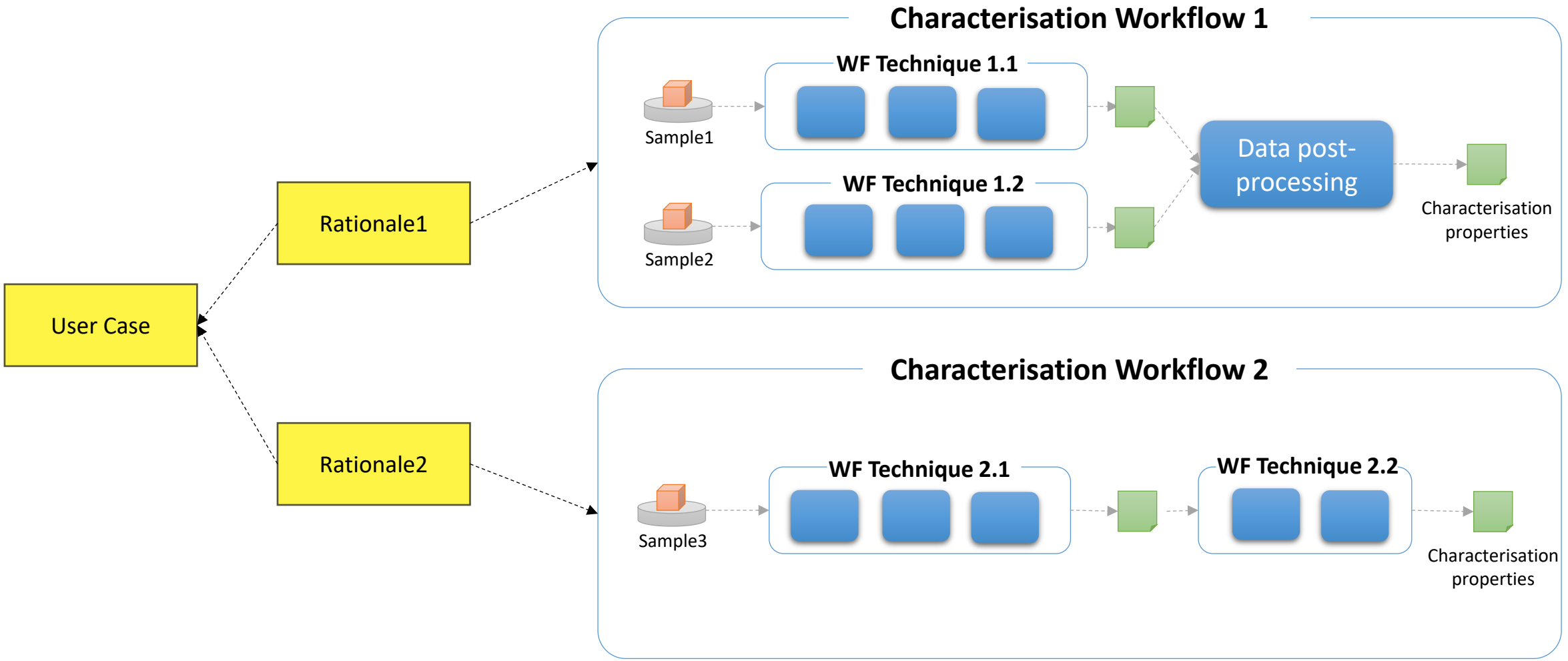
Ontology development and maintenance

- CHAMEO is continuously updated and aligned with the work done in the CWA, with new classes, new relationships and various refinements.

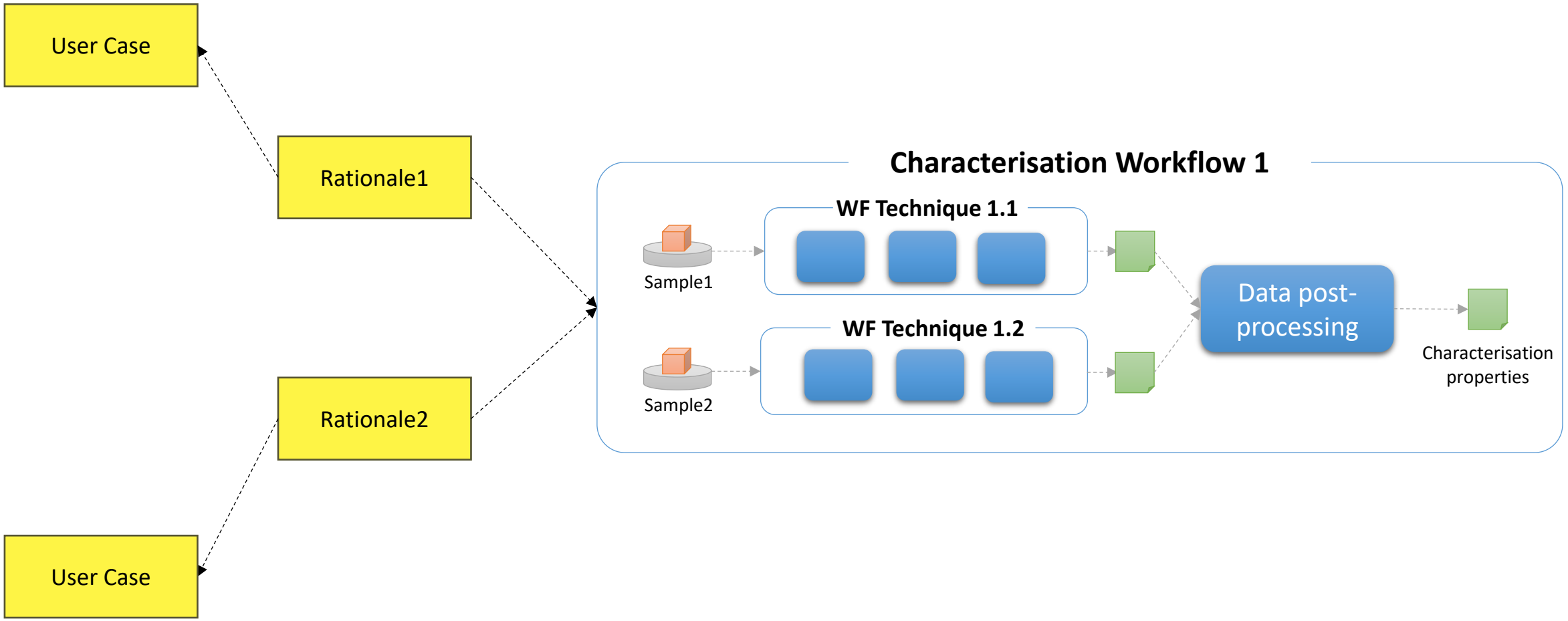
New CHADA based on the CHAMEO template



Same User Case with multiple Solutions



Same Solution for multiple User-cases



CHAMEO (and related ontologies) papers

Battery testing ontology: An EMMO-based semantic framework for representing knowledge in battery testing and battery quality control — 2025
P Del Nostro, G Goldbeck, F Kienberger, M Moertelmaier, A Pozzi, ...
Computers in Industry 164, 104203

Nanoindentation Ontology: Harmonising knowledge and data for nanoindentation — 2024
P Del Nostro, D Toti, E Rossi, M Sebastiani, G Goldbeck
MecaNano, 2024

Review and Alignment of Domain-Level Ontologies for Materials Science — 2023
A De Baas, P Del Nostro, J Friis, E Ghedini, G Goldbeck, IM Paponetti, A Pozzi, A Sarkar, Lan Yang, FA Zaccarini, Daniele Toti
IEEE Access 11, 120372-120401

Modeling experts, knowledge providers and expertise in Materials Modeling: MAEO as an application ontology of EMMO's ecosystem — 2023
P Del Nostro, G Goldbeck, A Pozzi, D Toti
Applied Ontology, 1-20

The CHAMEO Ontology: Exploiting EMMO's Multiperspective Versatility for Capturing Materials Characterization Procedures. — 2022
P Del Nostro, G Goldbeck, D Toti
FOMI, 2022

CHAMEO: An ontology for the harmonisation of materials characterisation methodologies — 2022
P Del Nostro, G Goldbeck, D Toti
Applied Ontology 17 (3), 401-421

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GOLDBECK CONSULTING

NanoMECommons Open Day

Cambridge, 20 November 2024

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Thank you!

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