MatCHMaker
Materials Characterisation & Modelling

CHADA template for scanning electron microscopy and how to represent it in the knowledge base

and how to simplify the data documentation process

Jesper Friis, Francesca Bleken (SINTEF),
Elisabeth Thronsen , Sigurd Wenner (SINTEF)
Geoffrey Daniel (CEA)
Alexandre Ouzia (HM)

MatCHMaker

Objectives

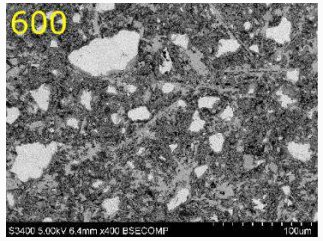
- **Accelerate advanced materials development**
  Including design, va
- **Reinforce traceabi**
  Integration of characterisation and mod ing data and workflows
- **Develop an open data repository**
  Based on semantics to connect desi and manufacturing processes

Documenting a characterisation workflow for cement

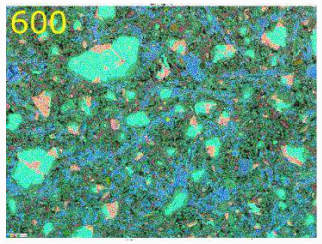
Use cases

- **Cement**: *Faster development of novel recycled low-carbon cement pastes*
- **Solid Oxide Fuel Cells**
- **Proton-Exchange Membrane Fuel Cells**

SEM characterisation of cement



Back-scattered electron (BSE) image



EDS elemental map

Sample	C	O	Na	Mg	Al	Si	S	Cl	K	Ca	Ti	Fe	CaSiAl	Ca/CaSiAl	Si/CaSiAl	Al/CaSiAl
600	27.31	46.59	0.98	0.84	2.65	4.33	0.58	0.15	0.71	15.33	0.05	0.48	22.31	69	19	12
601	23.16	50.69	2.52	0.75	2.05	4.06	0.51	0.09	1.80	13.90	0.05	0.42	20.01	69	20	10
602	29.22	47.00	0.14	0.56	5.14	6.66	0.71	0.15	0.21	9.45	0.08	0.67	21.25	44	31	24
603	32.29	45.42	0.15	0.48	4.35	7.64	0.64	0.15	0.24	7.98	0.08	0.60	19.97	40	38	22
604	41.23	41.62	0.24	0.54	0.50	2.09	0.50	0.22	0.50	12.34	0.03	0.20	14.93	83	14	3
605	37.15	44.34	0.13	0.66	0.64	2.04	0.61	0.22	0.24	13.73	0.02	0.23	16.41	84	12	4
606	25.41	47.71	0.19	0.57	1.37	5.03	0.74	0.16	0.39	17.60	0.05	0.76	24.00	73	21	6
607	18.66	53.33	0.15	0.57	1.27	5.30	0.66	0.09	0.86	18.34	0.05	0.71	24.91	74	21	5
608	36.13	43.26	0.05	0.29	3.46	6.19	0.66	0.18	0.12	8.96	0.08	0.65	18.61	48	33	19
609	31.84	47.03	0.00	0.32	2.88	6.61	0.72	0.16	0.16	9.42	0.08	0.78	18.91	50	35	15
610	13.75	55.25	0.00	0.69	1.49	6.06	0.56	0.05	0.53	19.70	0.06	0.84	27.25	72	22	5
611	19.29	52.13	0.63	1.07	1.41	5.12	0.71	0.07	1.16	17.79	0.06	0.55	24.32	73	21	6
AVG	24.18	49.95	0.17	0.59	1.98	5.72	0.68	0.12	0.54	15.30	0.06	0.72	23.00	65.06	25.62	9.32

Quantified elemental map

Phases	Phase fraction
Phase 1	0.21
Phase 2	0.32

Cement paste phase fractions

Sample extraction & preparation → SEM measurement → Data processing → Result analysis

Common standard for documenting characterisation workflows (CHADA)

CEN Workshop Agreement (CWA 17815)

Definition of terms

3.6

characterisation data post-processing

data analysis and transformation that allows to calculate the material property/behaviour from the calibrated primary data.

Note 1 to entry Characterisation data post-processing involves the application of a method, based on some theory or model, to primary data to calculate the secondary data that provide the information about the characterisation property or behaviour.

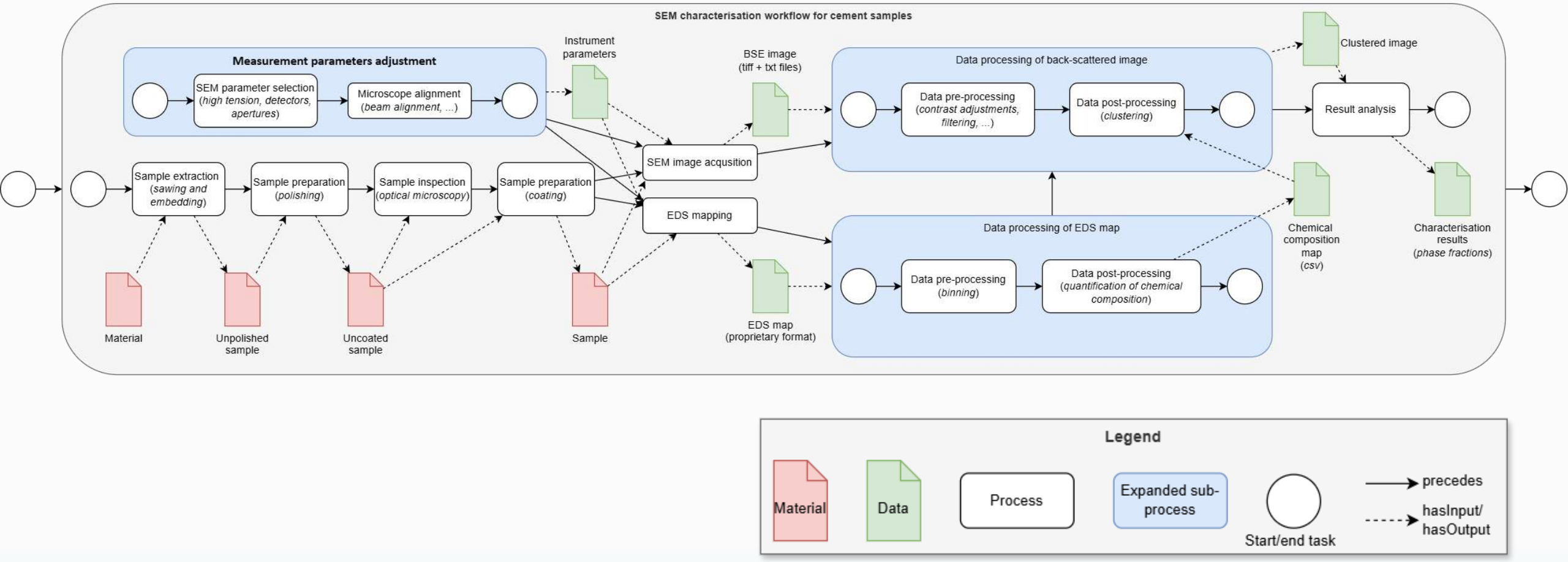
Note 2 to entry Characterisation data post-processing includes digital image processing to enhance or extract useful information.

EXAMPLE 1 In nanoindentation testing, the Oliver-Pharr method is used, which allows calculating the elastic modulus and hardness of the sample by using the load and depth measured signals.

EXAMPLE 2 Analysis of Scanning Electron Microscopy (SEM) (or optical) images to gain additional information, for example microstructural analysis, grain size evaluation, digital image correlation procedures.

Documenting SEM characterisation of cement

BPMN diagram of the workflow



CHADA

A structured way to document a characterisation workflows

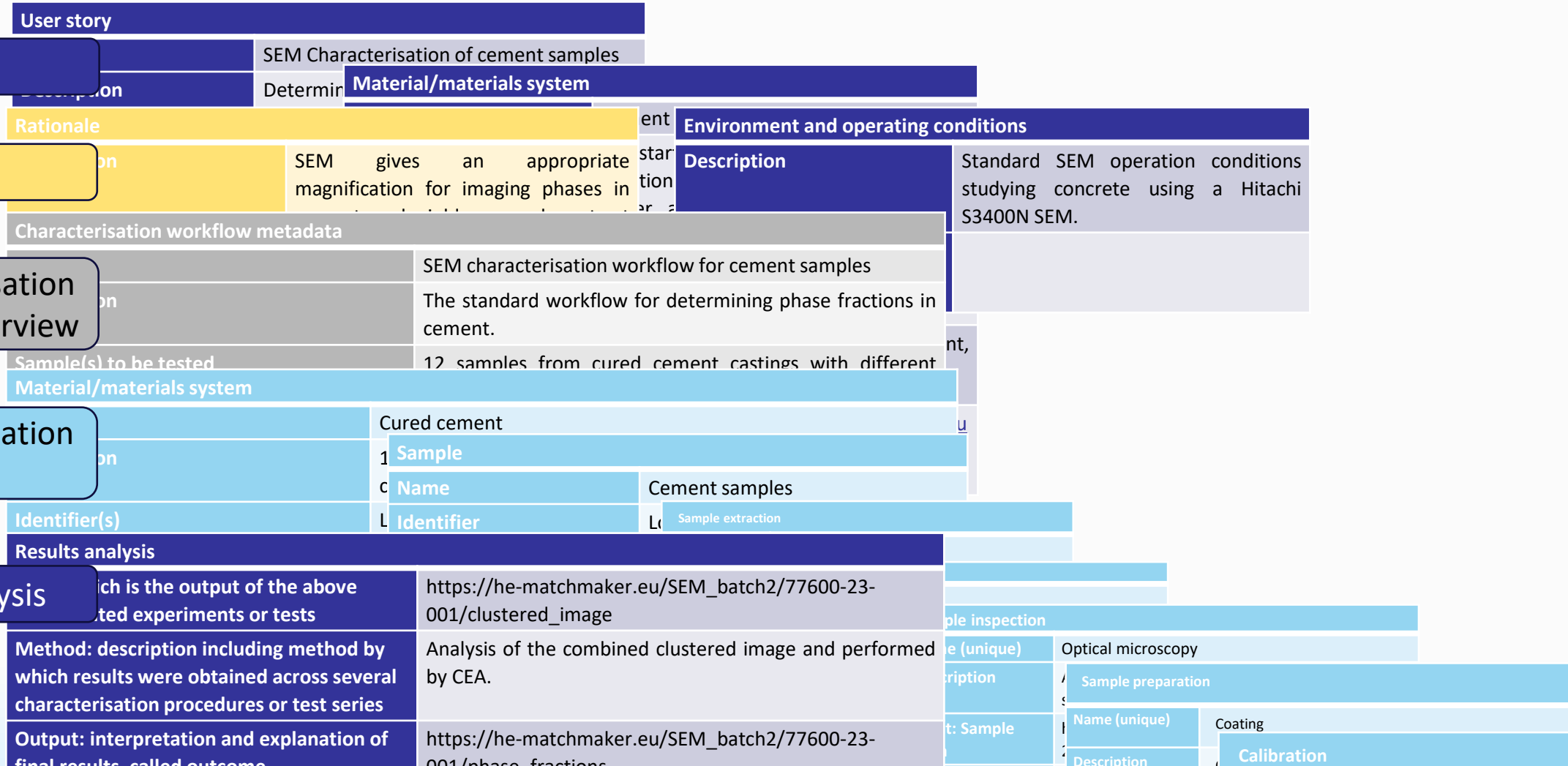
1. User story

2. Rationale

3. Characterisation workflow overview

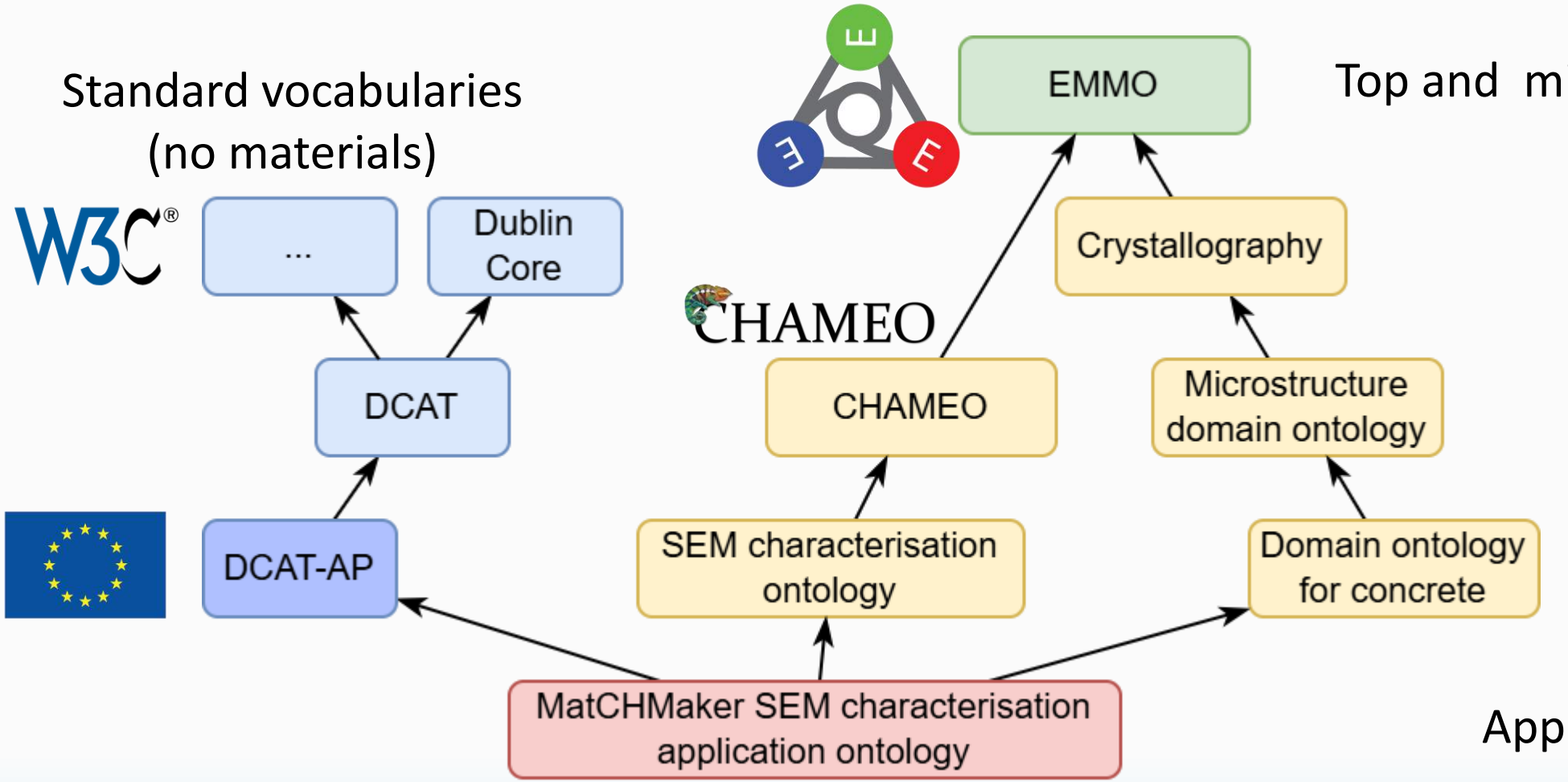
4. Characterisation case

5. Result analysis

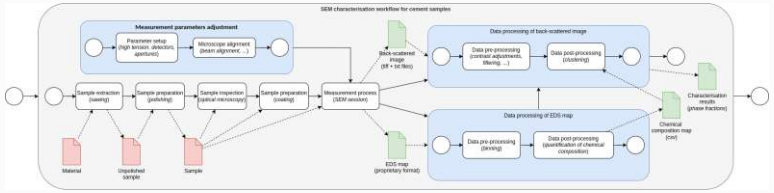


…very nice, but not machine readable

Standard vocabularies
(no materials)



Representing the workflow semantically



BPMN diagram

CHADA tables (not machine readable)

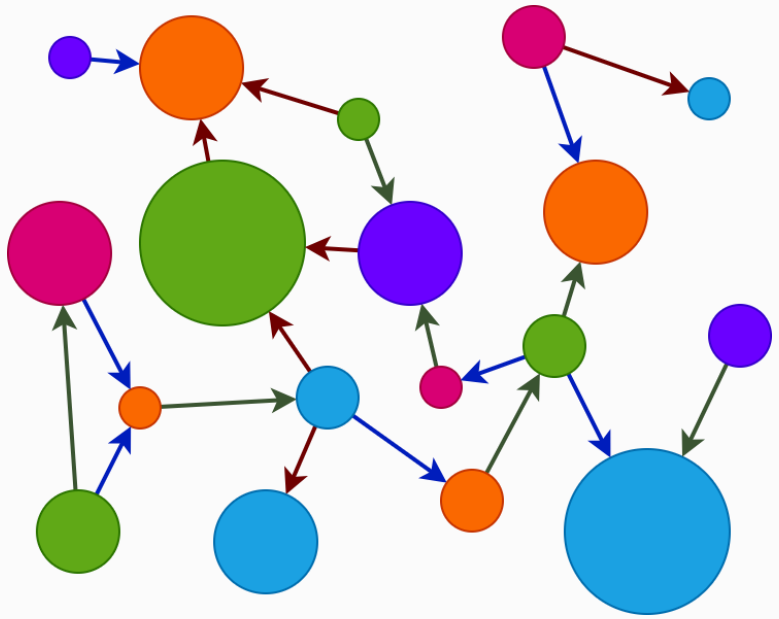
methodology & tools

Developed in MatCHMaker, +++

DLite

TRIPPER

EMMOntoPy



Knowledge base representation

Representing the workflow

Demo at:
https://github.com/HEU-MatCHMaker/DataDocumentation/tree/master/examples/CHADA-workflow

Datasets

	@id	@type	@type	title	description	theme	publisher.name	contactPoint.hasName	distribution.downloadURL	distribution.mediaType
2	:bse_image	dcat:Dataset	http://onto-ns.com/meta/matchmaker/0.2/SEMImage	BSE image	Back-scattered SEM image of sement sample	SEM	MatCHMaker	Sigurd Wenner		https://www.iana.org/assignments/media-types/image/tiff
3	:eds_map	dcat:Dataset	http://onto-ns.com/meta/matchmaker/0.2/SEMImage	EDS map	EDS map of sement sample	SEM	MatCHMaker	Sigurd Wenner		https://www.iana.org/assignments/media-types/application/vnd.hitachi
4	:chem_comp_map	dcat:Dataset	http://onto-ns.com/meta/matchmaker/0.2/SEMImage	Chemical compositon map	Chemical composition map extracted from EDS map	SEM	MatCHMaker	Sigurd Wenner		https://www.iana.org/assignments/media-types/text/csv
5	:phase_fractions	dcat:Dataset	http://onto-ns.com/meta/matchmaker/0.2/SEMImage	Phase fractions	Relative amount of the different phases in the sement	SEM	MatCHMaker	Sigurd Wenner		https://www.iana.org/assignments/media-types/application/vnd.ms-excel

Processes

	@id	@type	title	description	theme
2	:sem_characterisation	chameo:CharacterisationProcedure	SEM characterisation	SEM characterisation workflow of cement samples	SEM
3	:sample_extraction	chameo:SampleExtraction	Sawing	Extraction of SEM sample from the casted sement by sawing	SEM
4	:sample_preparation1	chameo:SamplePreparation	Polishing	Polishing the extracted SEM sampe	SEM
5	:sample_inspection	chameo:SampleInspection	Optical microscopy	Sample inspection by optical microscopy	SEM
6	:sample_preparation2	chameo:SamplePreparation	Coating	Coating the SEM sample with carbon to make it electrical conducting	SEM
7	:sem_alignment	chameo:MeasurementSystemAdjustment	SEM alignment	Measurement parameter adjustment	SEM
8	:parameter_setup	chameo:MeasurementSystemAdjustment	SEM parameter setup	Select high tension, detectors, apartures, etc	SEM
9	:beam_alignment	chameo:MeasurementSystemAdjustment	Beam alignment	Align the electron beam.	SEM
10	:measurement_process	chameo:CharacterisationMeasurementProcess	SEM Measurement process	Acquire BSE images and EDS maps	SEM
11	:bse_processing	chameo:DataProcessing	Processing of BSE image	Processing of back scattered image	SEM
12	:bse_preprocessing	chameo:DataPreparation	BSE pre-processing	Filter the BSE image and adjust contrast.	SEM
13	:bse_postprocessing	chameo:DataPostProcessing	BSE clustering	Cluster the combined BSE image and EDS map	SEM
14	:eds_processing	chameo:DataProcessing	Processing of EDS map	Processing of EDS map	SEM
15	:eds_preprocessing	chameo:DataPreparation	EDS binning	Pre-process EDS map by binning.	SEM
16	:eds_postprocessing	chameo:DataPostProcessing	EDS quantification	Use EDS map to quantify chemical composition.	SEM

Materials

	@id	@type	title	description	theme
2	:material	emmo:Material	Cement	Cement casting.	SEM
3	:unpolished_sample	@chameo:Sample	Unpolished sample	Unpolished SEM sample from cured cement paste.	SEM
4	:sample	@chameo:Sample	Sample	SEM sample from cured cement paste.	SEM

Representation in the knowledge base

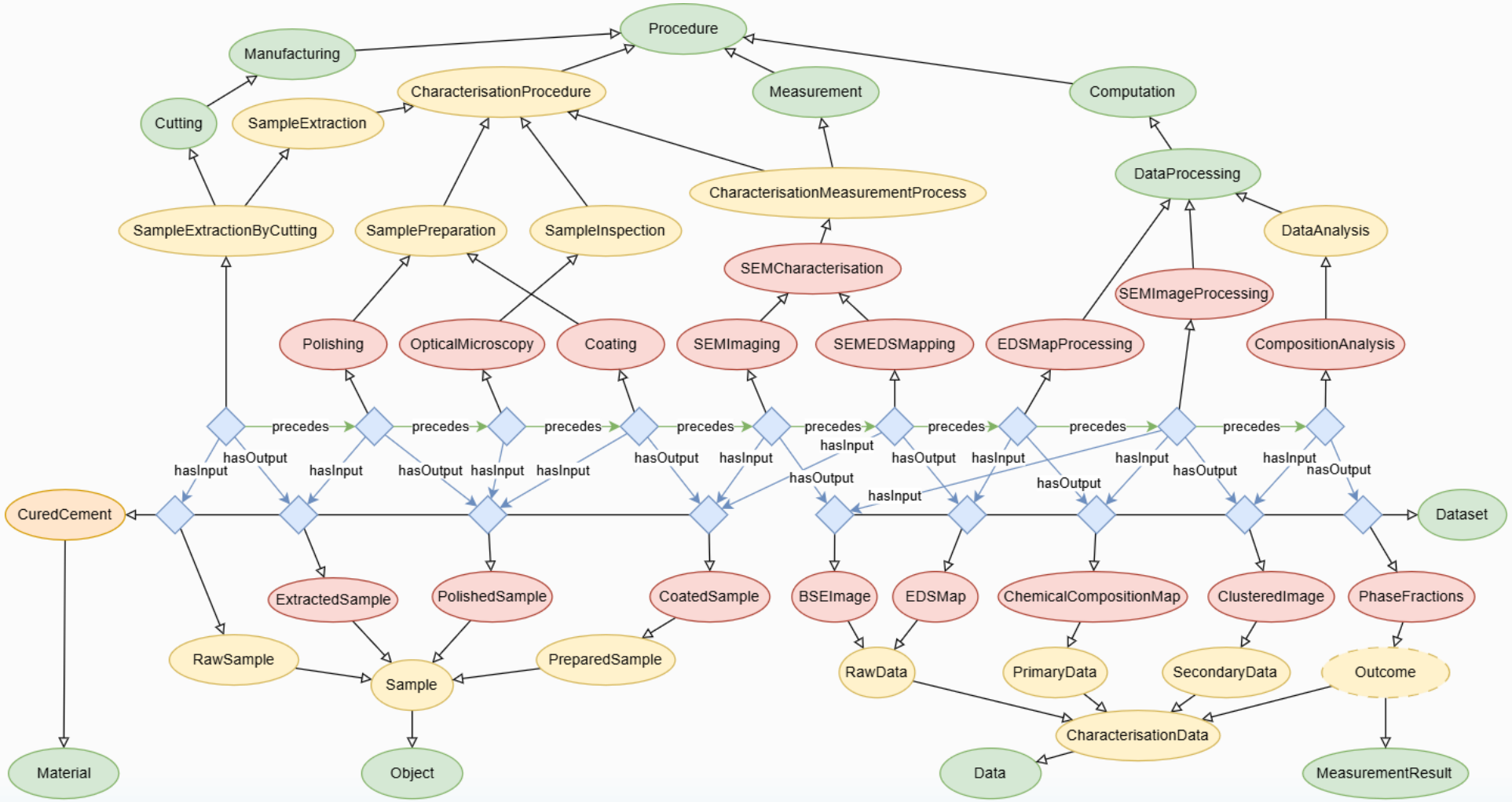
EMMO

CHAMEO

Domain ontology for Concrete

SEM characterisation ontology

Individuals

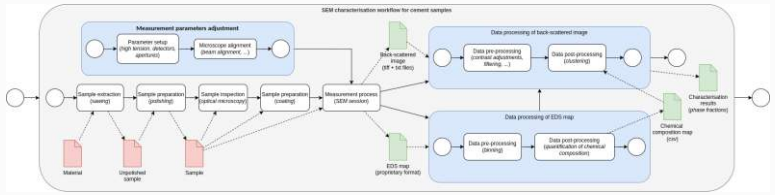


Further work: simplifying the documentation process even more

See also the poster by Francesca L. Bleken

- Repeating these tables for each characterisation session is tedious
- Repetition can be reduced/eliminated by generalisation
  - Document procedures once in the application ontology (fully annotated)
  - Workflow from BPMN diagram (xml)
  - When executed, automatically populate the KB with individuals

Application ontology (semantically annotated)

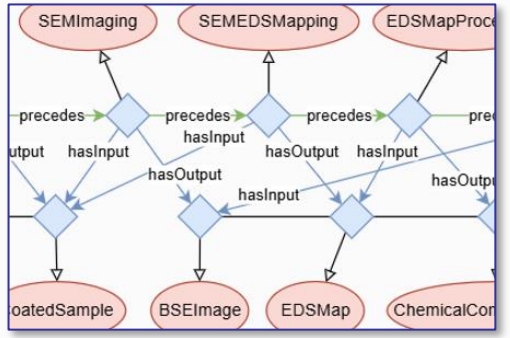


BPMN diagram (xml)

execution

tooling

KB: automatically populated with individuals



Acknowledgement

We kindly acknowledge funding from the European Union‘s Horizon 2020 and Horizon Europe research and innovation programs and the Norwegian Research Council via the following projects:

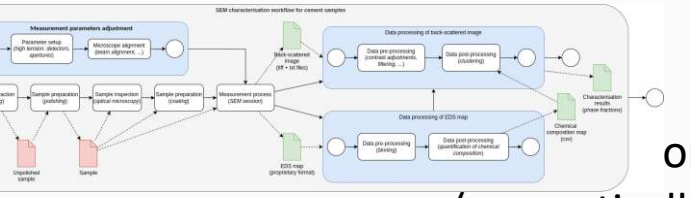
- MatCHMaker (2022-2026) Grant Agreement n. 101091687
- OntoTrans (2020-2024) Grant Agreement n. 862136
- SFI PhysMet (2020-2028) Research Council of Norway n. 309584
- OpenModel (2021-2025) Grant Agreement n. 953167
- NanoMECommons (2021-2025) Grant Agreement n. 952869
- PINK (2024-2028) Grant Agreement n. 101137809

Ongoing work: further simplifying the documentation process

See also the poster by Francesca L. Bleken

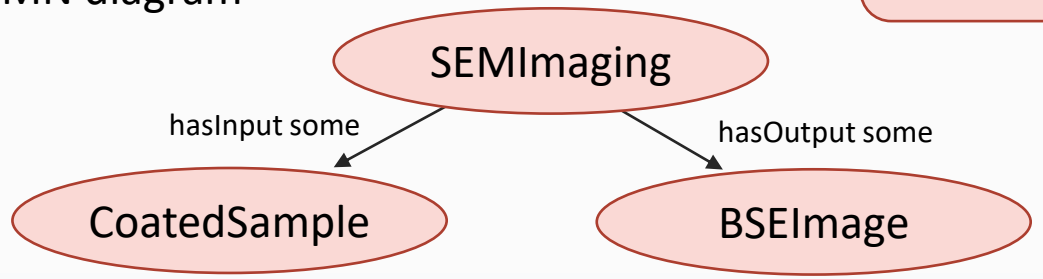
- Repeating these tables for each characterisation session is tedious
- Repetition can be reduced/eliminated by generalisation

  Document procedures once in the application ontology (fully annotated)
  Workflow from BPMN diagram (xml)
  When executed, automatically populate the KB with individuals



BPMN diagram

on ontology
(semantically annotated)



Application ontology
(semantically annotated)

execution

tooling

Annotated individuals
and relations between them