1. YOUR NAME AND NAME OF YOUR TAXONOMY AND/OR ONTOLOGY

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Name of the Ontology/Taxonomy:

ONTOLOGY/TAXONOMY FOR MATERIALS CHARACTERISATION, including (at this stage):

Documentation of Characterisation Data (CHADA)

Classification of Characterisation methods

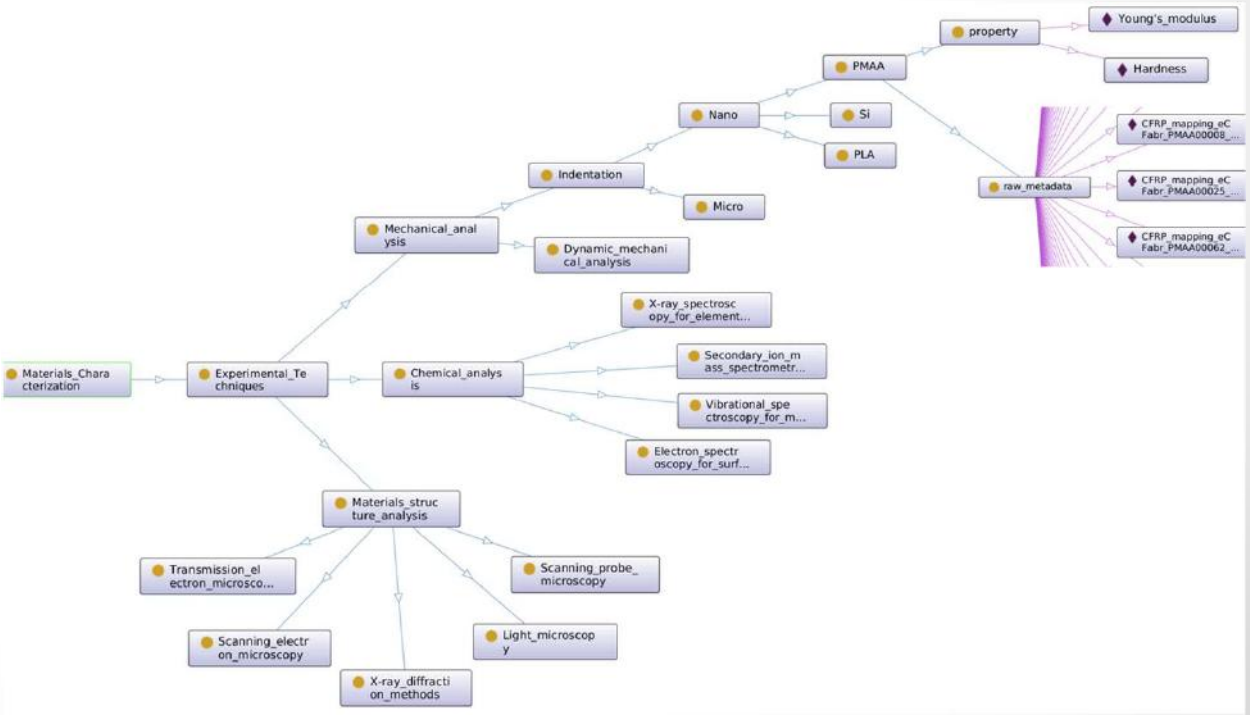
Taxonomy for nano-scale mechanical characterisation

2. What is the application domain of your taxonomy and/or ontology?

Experimental Characterisation of materials.

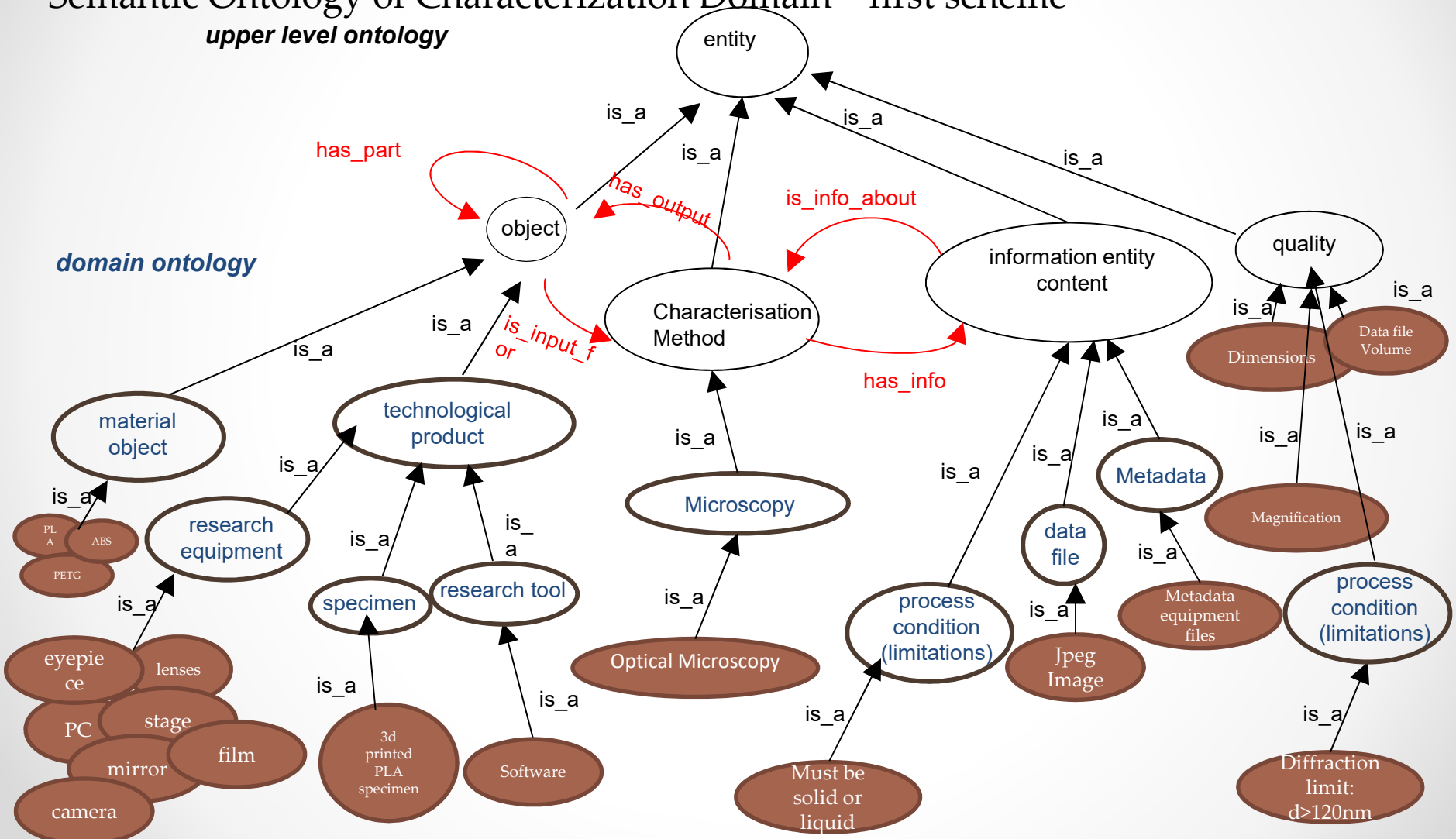
Using some of the resources within the H2020 project OYSTER, we are developing the initial steps for taxonomy and ontology in materials characterisation.

In OYSTER, we will develop the Data Documentation Scheme (CHADA) and a taxonomy and the specific ontology for ONE class of characterisation method (namely, nanoindentation).



2. What is the application domain of your taxonomy and/or ontology?

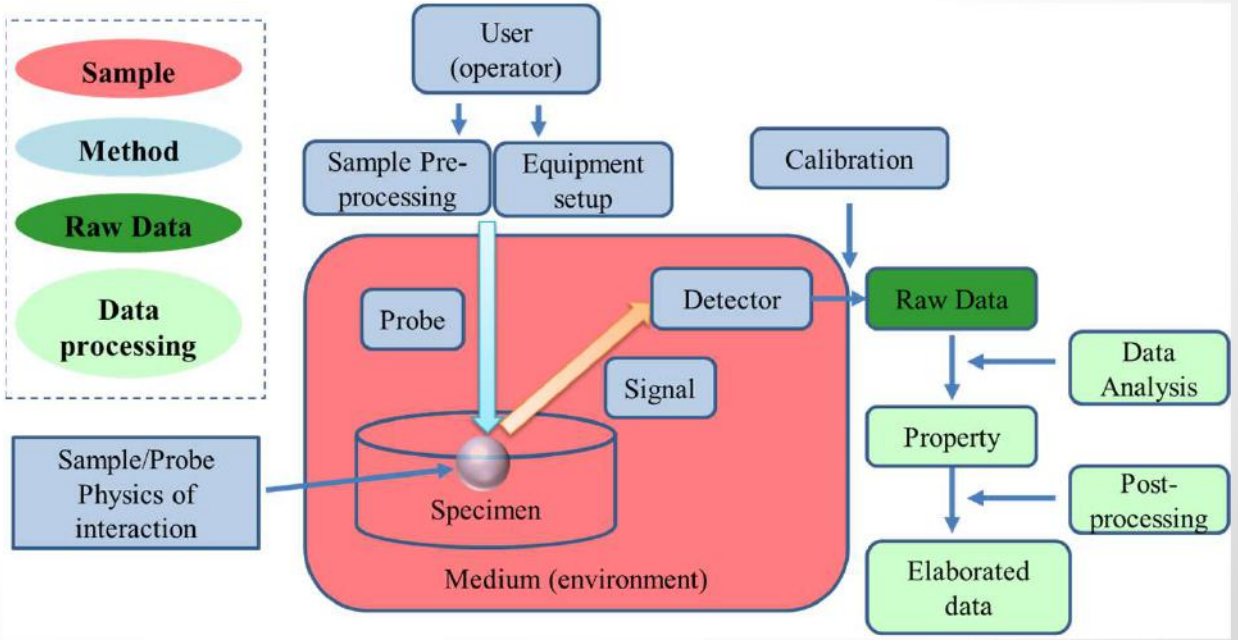
Semantic Ontology of Characterization Domain – first scheme



3. WHAT IS THE INTENDED PURPOSE OF THE TAXONOMY AND/OR ONTOLOGY?

Developing a standard and interoperable format and structure for materials characterisation data.

Data from experimental characterisation can be very different. However, we found that a standard scheme could be developed if one starts from the definition of the basic vocabulary and the connections among a set of relevant keywords. The first representation of a generic characterisation experiment was already developed and published:



https://www.preprints.org/manuscript/201903.0205/v3

4. What is the representation language and implementation (logics)?

Initial workflows and docx templates for CHADA have been already developed (see links below).
The related ontology will be built entirely on the basis of the EMMO structure (under supervision, in OYSTER, of Gerhard Goldbeck and Adham Hashibon).

Main Introduction to the CHADA concept and case studies:	https://zenodo.org/record/2636609
CHADA docx detailed forms:	https://zenodo.org/record/2637419
Data Management Plan with CHADA workflow sheet embedded:	https://zenodo.org/record/2636533

5. WHAT IS THE KNOWLEDGE YOUR SPECIFIC TAXONOMY AND/OR ONTOLOGY REPRESENTS?

a) **Knowledge necessary for a pragmatic description of current practices**

Current practices of experimental materials characterisation are based on the knowledge of the proto-to-sample physics of interaction and the analytical (or numerical) data based rules for analyzing the raw signal (raw data) for extraction of the main properties of interest.

a) **Explanation of the world according to one of the philosophical views called realism/conceptualism/nominalism**

Nominalist – The taxonomy that is being developed (and the ontology later on) is based on the concept that a a property is always the result of a measurement.

6. How does your taxonomy and/or ontology represent granularity?

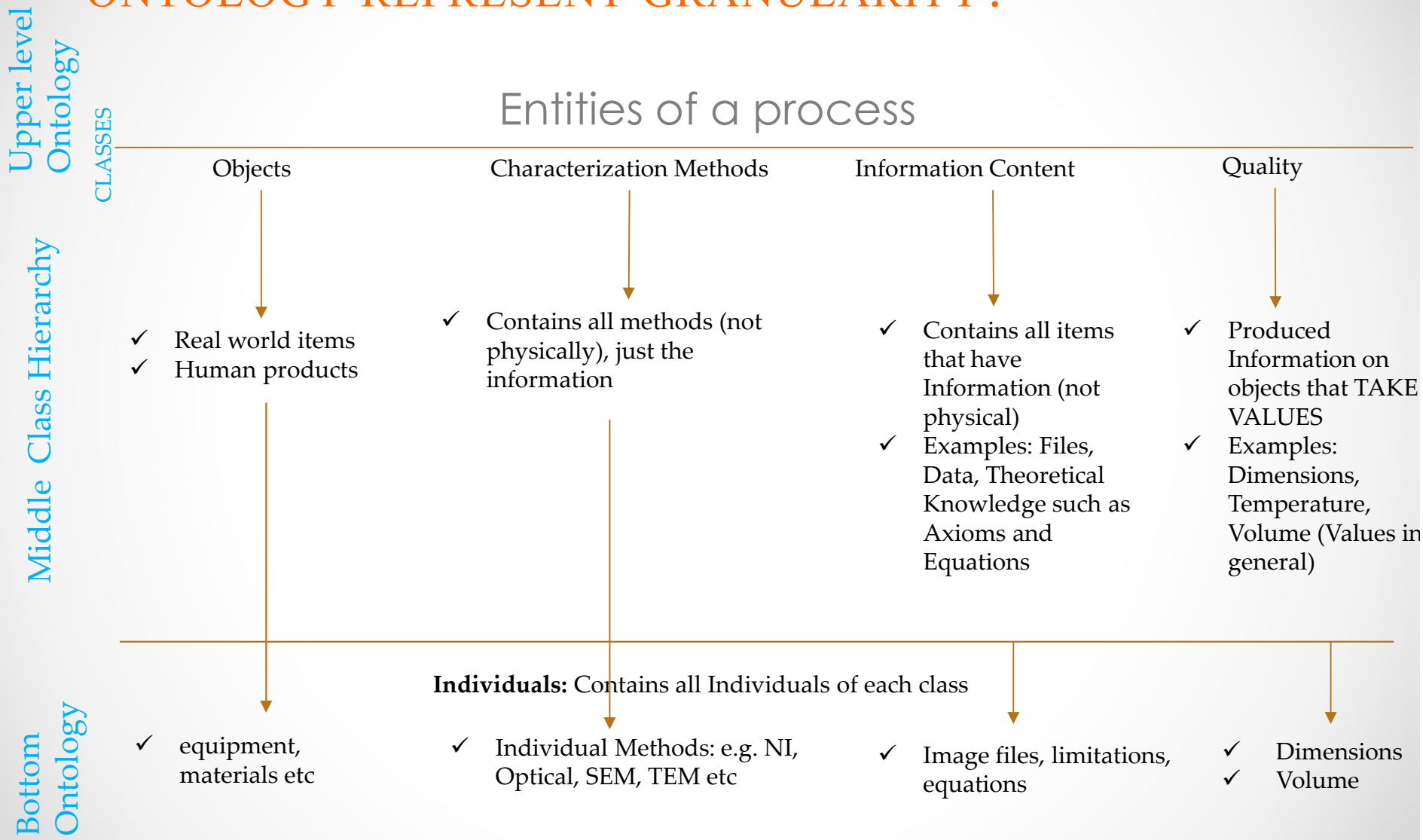
Materials characterisation can be MULTISCALE by definition, depending on the characteristic VOLUME OF INTERACTION between the probe and the sample and the REPRESENTATIVE VOLUME ELEMENT (RVE).

There are techniques that describe the RVE as a continuum, whilst other methods (sometime based on the same physics of interaction) can describe it as discrete particles or by quantum mechanics.

Linking across scales in materials characterisation will be done using the concept of RVE.

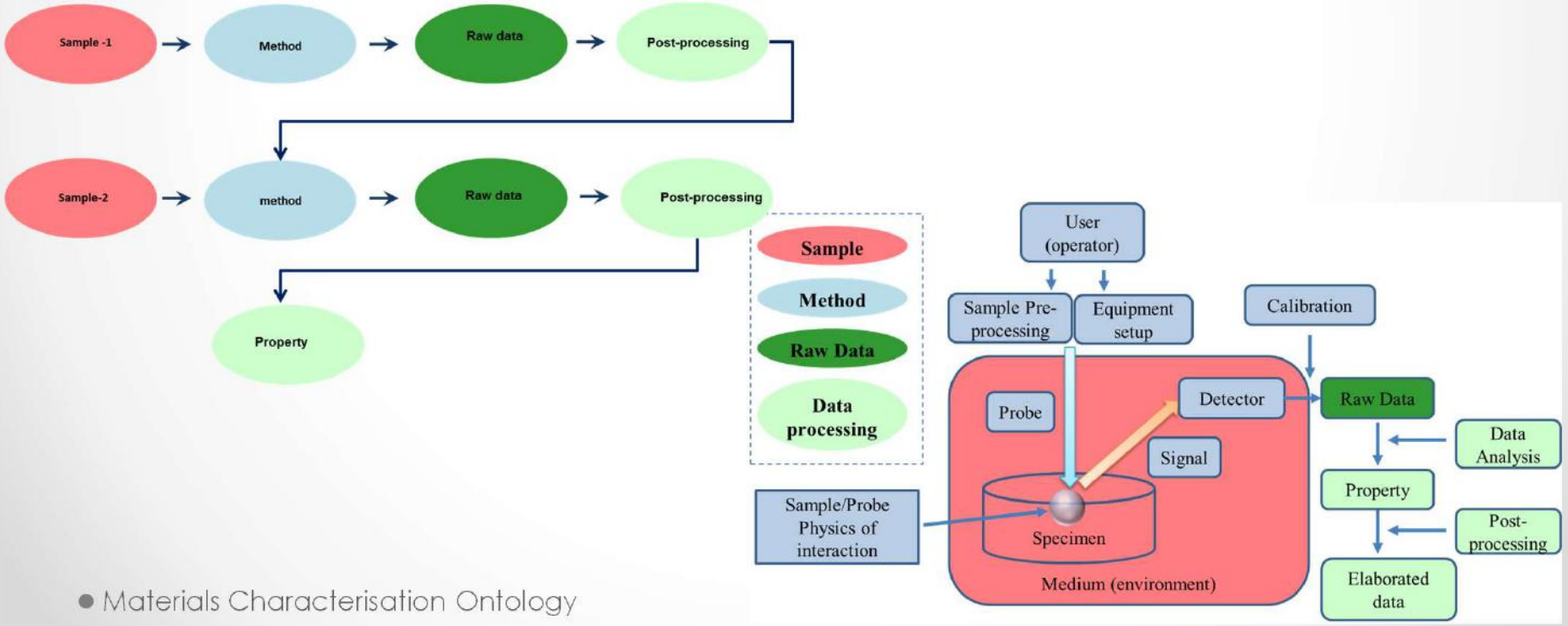
However, most of the characterisation methods for applications in nanotechnology and nano-medicine use a continuum description of the RVE.

6. How does your taxonomy and/or ontology represent granularity?



7. How does your taxonomy and/or ontology represent processes?

- Our approach is currently only aimed at a classification and analytic description of characterisation “WORKFLOWS” (which represent the main “processes” under investigation).
- In the taxonomy (and ontology) under development, a process will be represented by the evolution of a characterisation workflow with time (where not only the sample, but also the probe, could change with time).



● Materials Characterisation Ontology

8. How does your taxonomy and/or ontology capture materials?

In the field of characterisation, a MATERIAL is captured only in terms of the characteristic sample volume, which represent the volume of interaction between the sample and the experimental probe.

9. How does your taxonomy and/or ontology capture manufacturing?

In the characterisation ontology being developed, a LINK will be created among each class of characterisation methods AND the Manufacturing Processes AND the materials that can be characterized through that method.

In example, x-ray diffraction can be associated to crystalline material and to those processes to fabricate crystalline materials (e.g. metallurgical processes, 3D printing of metals, MEMS fabrication, thin film synthesis, etc.)

10. How does your taxonomy and/or ontology address the circle connection between physical properties, materials models (see definition in RoMM Review of Materials Modelling VI) and measurement?

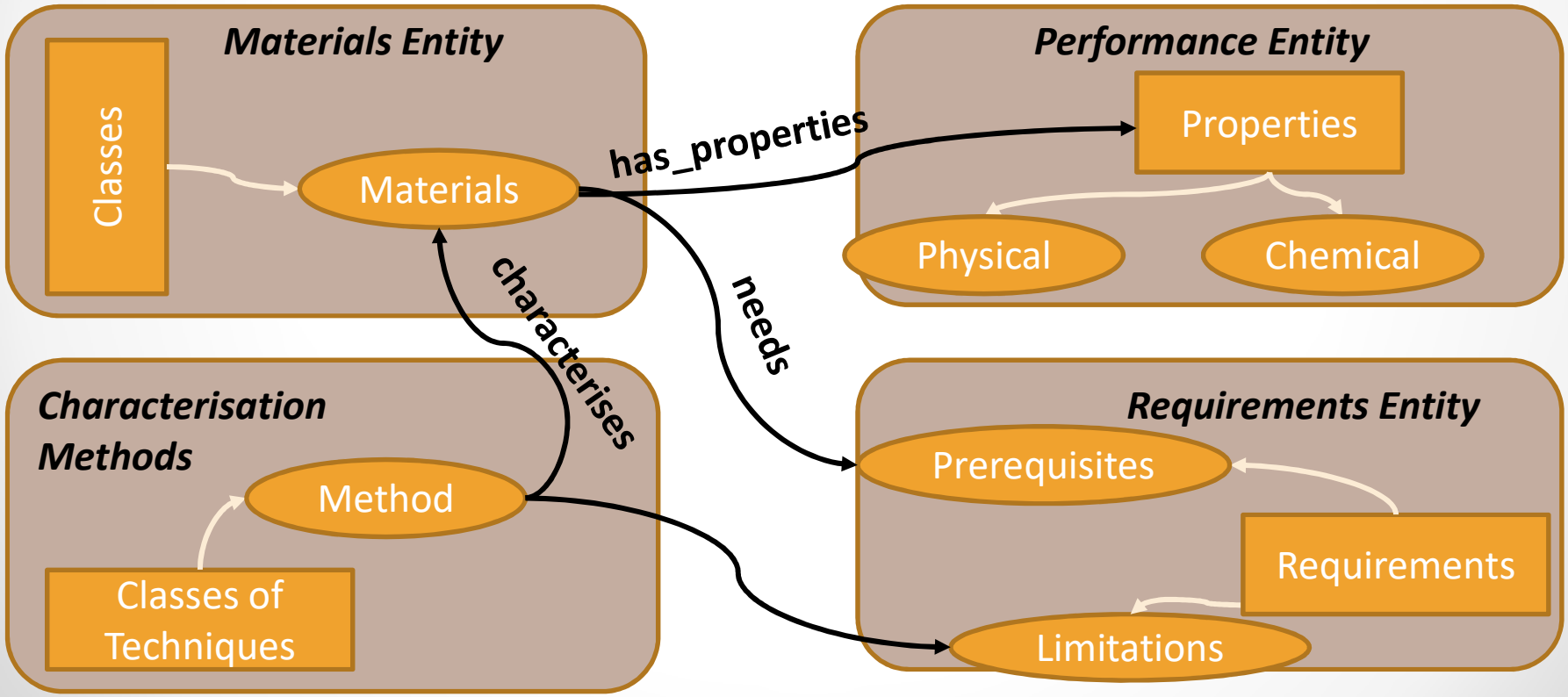
Materials characterisation represents the experimental cornerstone for validation of models and quantification of the physical properties.

In a materials characterisation taxonomy and/or ontology, each characterisation method will be LINKED to those physical properties that can be measured by that method and to Materials models that can simulate that method. Therefore, the basis will always be the method, and then the taxonomy and/or ontology will establish a keyword/based technologies with the properties and models.

Example in next slides.

10. How does your taxonomy and/or ontology address the circle connection between physical properties, materials models (see definition in RoMM Review of Materials Modelling VI) and measurement?

Example: Method **TEM** of the Class **Microscopy** characterises **Carbon Nanotubes** of the **Class Nanomaterials**. CNTs have **Tensile Strength** of 13GPa and require a protection layer (**Prerequisite**) to avoid deterioration. **TEM** has the limitation of <100 nm specimen' thickness.



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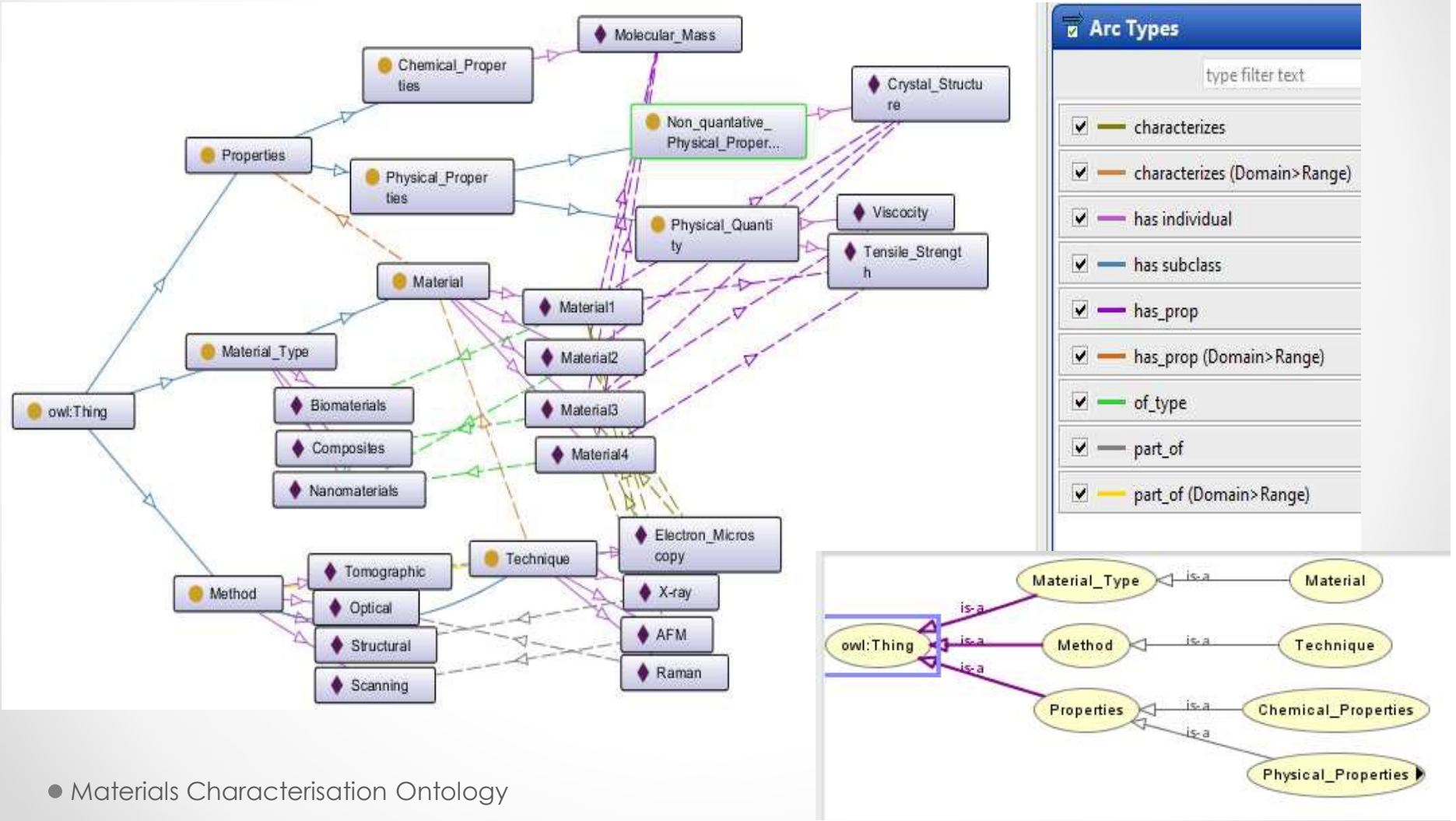
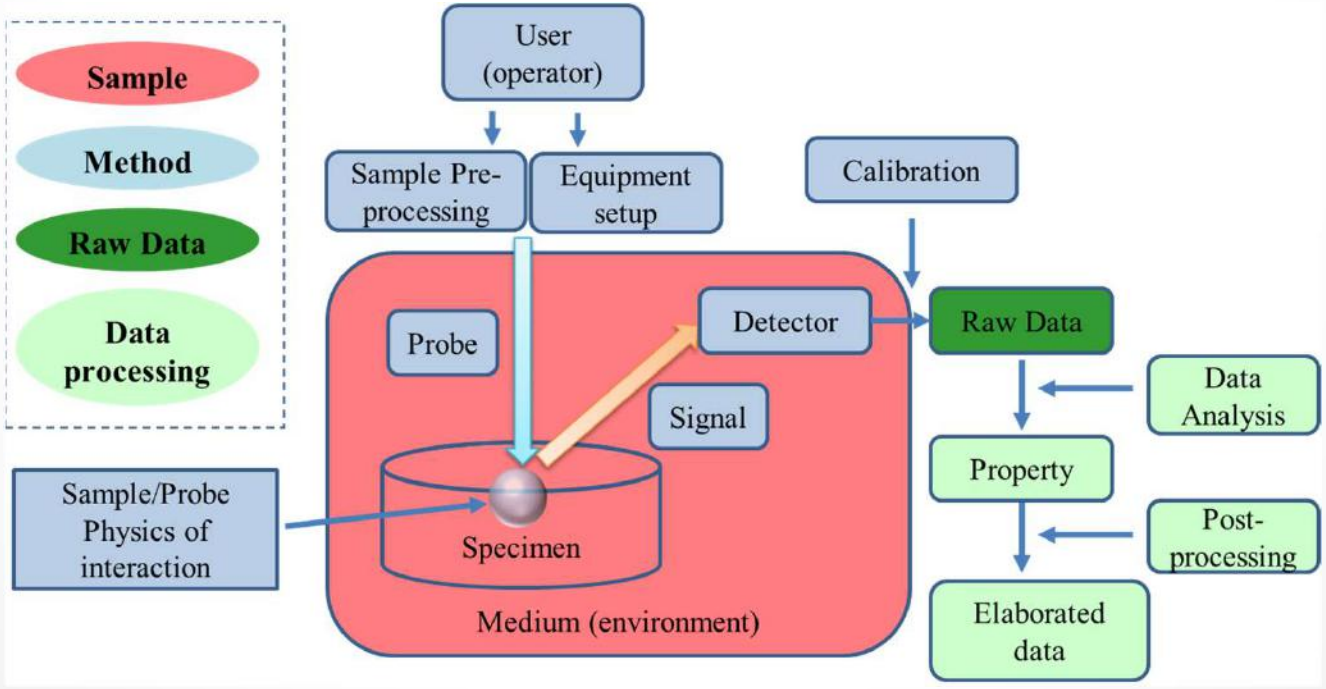


- Materials Characterisation Ontology

11. WHAT ARE THE CONCEPTS, WITH DEFINITIONS, IN THE UPPER LEVEL OF YOUR TAXONOMY AND/OR ONTOLOGY?

These are the main concepts, keywords and correlations at the basis of our materials characterisation ontology:



12. WHAT ARE THE INDUSTRIAL USE CASES OF THE TAXONOMY AND/OR ONTOLOGY (E.G. IN ONTOLOGY-DRIVEN TOOLS)?

The USER-CASE developed in OYSTER is: nano-scale adhesion and surface-energy assessment in superhydrophobic materials.

13. What overlaps do you see with other taxonomy and/or ontologies?

Deep overlap, since the beginning, with EMMO action.

THANK YOU!

Acknowledgement:

The entire OYSTER team is currently contributing to development of CHADA, nanomechanical testing taxonomy and interaction with EMMO.