

# INTEGRATED COMPUTATIONAL/EXPERIMENTAL MATERIAL ENGINEERING OF THERMAL SPRAY COATINGS

**EMMO for Manufacturing: the CoBRAIN Knowledge  
Base for Thermal Spraying Process, Modelling and  
Characterisation**



MatCHMaker @ EMMC 2025 Satellite Workshop

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Presenters:

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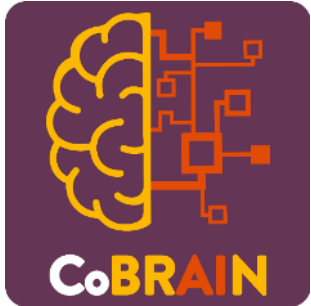


ALMA MATER STUDIORUM  
UNIVERSITÀ DI BOLOGNA



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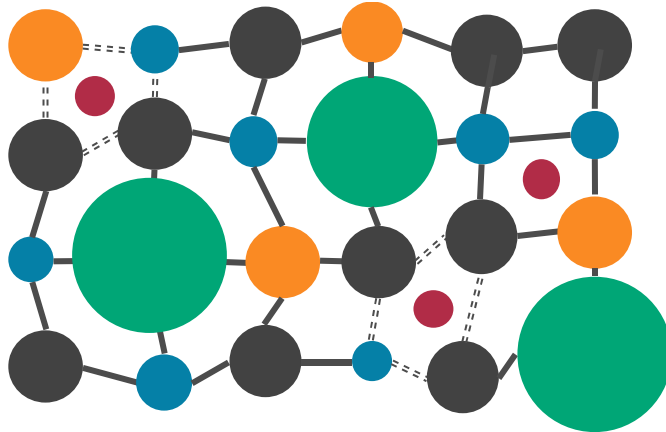
## INTEGRATED COMPUTATIONAL/EXPERIMENTAL MATERIAL ENGINEERING OF THERMAL SPRAY COATINGS

- **Protective coatings** against wear and corrosion play a critical role in strategic industrial fields
  - Extant technologies have considerable drawbacks in terms of sustainability
    - ✓ Electroplated Cr is a safe material, but its deposition involves the use of carcinogenic  $\text{Cr}^{6+}$  compounds subject to authorisation under REACH Annex XIV
    - ✓ Electroplated or electroless Ni(P) or Ni(B) based layers also use hazardous raw materials and result in coatings that might be less safe
    - ✓ Thermal spray WC-Co-based coatings utilize carcinogenic materials – Co – as well as critical raw materials (CRMs) – Co, W
- ⇒ **Identify novel formulations**, exploiting the versatility and low environmental impact of thermal spraying to produce alloy and hardmetal coatings free of toxic/critical materials.

# The Project



## High Entropy Alloys - HEA



## Materials space

Multi-principal element metal matrix and carbides

Elements for HEA metal binder

Al	Si	Ti	V	Cu
Cr	Mn	Fe	Ni	Co

Elements for hard phase

Ti	C	B	Nb	Mo
		Hf	Ta	W

126 equiatomic combinations of 4 or 5 elements  
62370 cermets (without composition optimization)

- **High-entropy effect**

Multi-element systems often consist of one (HEAs) or two main phases, instead of a wider range of binary or ternary solid solutions and intermetallics, because of the stabilizing effect of the large entropy of a multi-element random solid solution ( $\Delta G = \Delta H - T \cdot \Delta S$ )

- **Lattice strain effect**

The mismatch in atomic radii result in lattice distortions that increase strength

- **Sluggish diffusion effect**

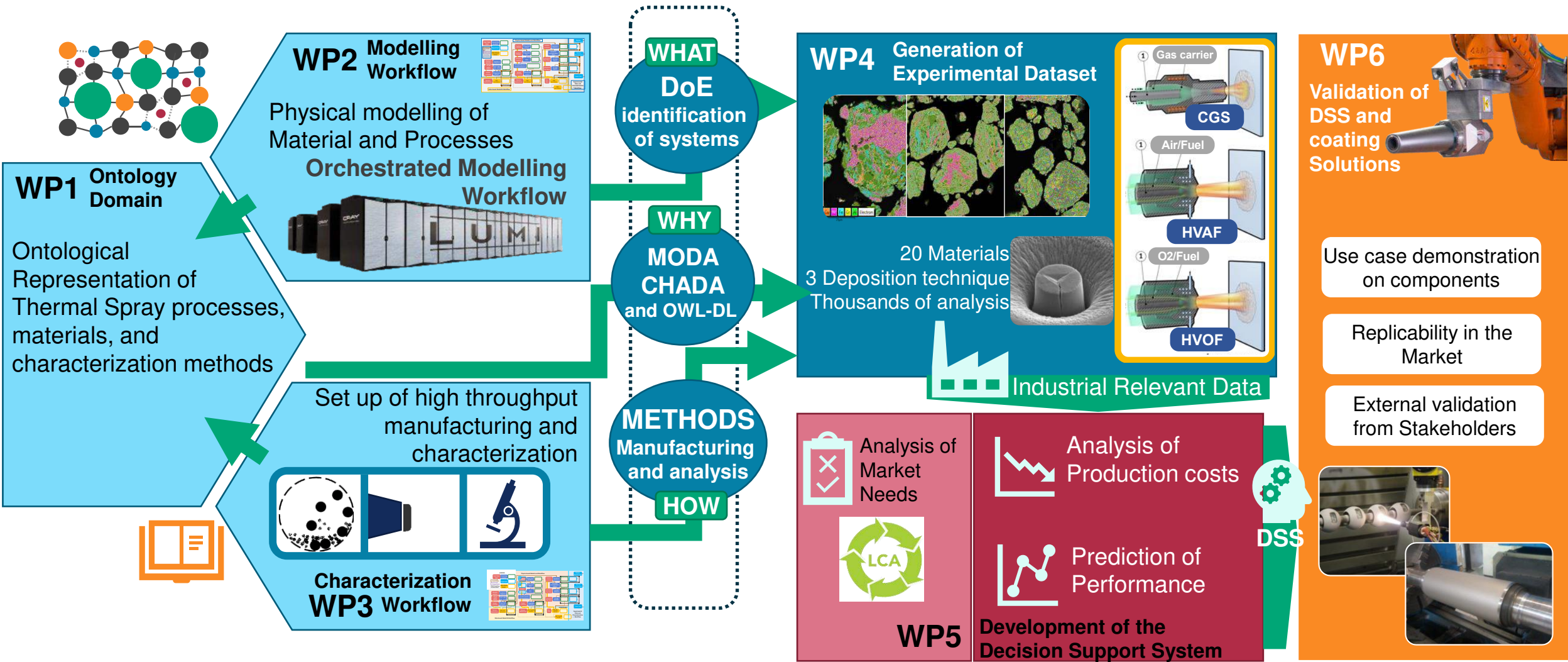
The distorted lattice hinders long-range diffusion, which also results in better high-temperature stability

- **“Cocktail” effect**

Non-linearities and unexpected synergistic effects may sometimes yield somewhat unpredictable outcomes

Need to combine experimental development, physical modelling & artificial intelligence

# The Project





# 1. Planning

- o Did they plan a priori which data they needed, and how to extract knowledge from it?
- o Did they work with Data Management Plans?



## CoBRAIN Data Management Plan

All datasets from **experiments**, **modelling** and **characterisation**, are documented in the DMP.

The tables are divided into **SHARED DATA** and **LOCAL DATA**:

**SHARED DATA and METADATA** Information that is uploaded in the CoBRAIN Knowledge Base: it has to be in the form of numerical or string values (rdfs:literal). For data which are not in the form of rdfs shareable values (i.e., images, XRD plots) quantitative values must be provided and/or its location specified using URIs or similar.

**LOCAL DATA** Information that is kept at partner premises: for these data a curator must be identified, and it is specified whether the data are openly shareable on request or confidential.

Nanoindentation - High speed 3D mapping

### SHARED DATA and METADATA

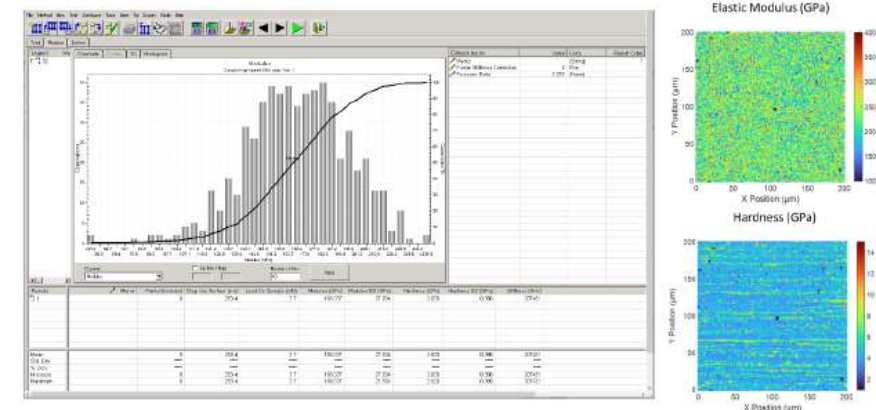
Field	Description
Sample ID	String: Sample name and identification number of test.
Sample description	String: sample composition and production information.
Test definition	String: Type of test and instrument name (i.e. Nanoindentation-High speed 3D mapping, MTS G200).
SOP file name	String: indication of the file name containing parameters of measurement (i.e. acquisition rate, max load, loading rate, approach speed etc.) .
Measurement Date Time	dd/mm/yyyy hh:mm:ss
Indenter	String: type of the indenter (i.e. Berkovich); serial number; material of the indenter
H, E maps	Data for 3D hardness and modulus maps (i.e. hardness value for x-y positions).

RDFS

### LOCAL DATA

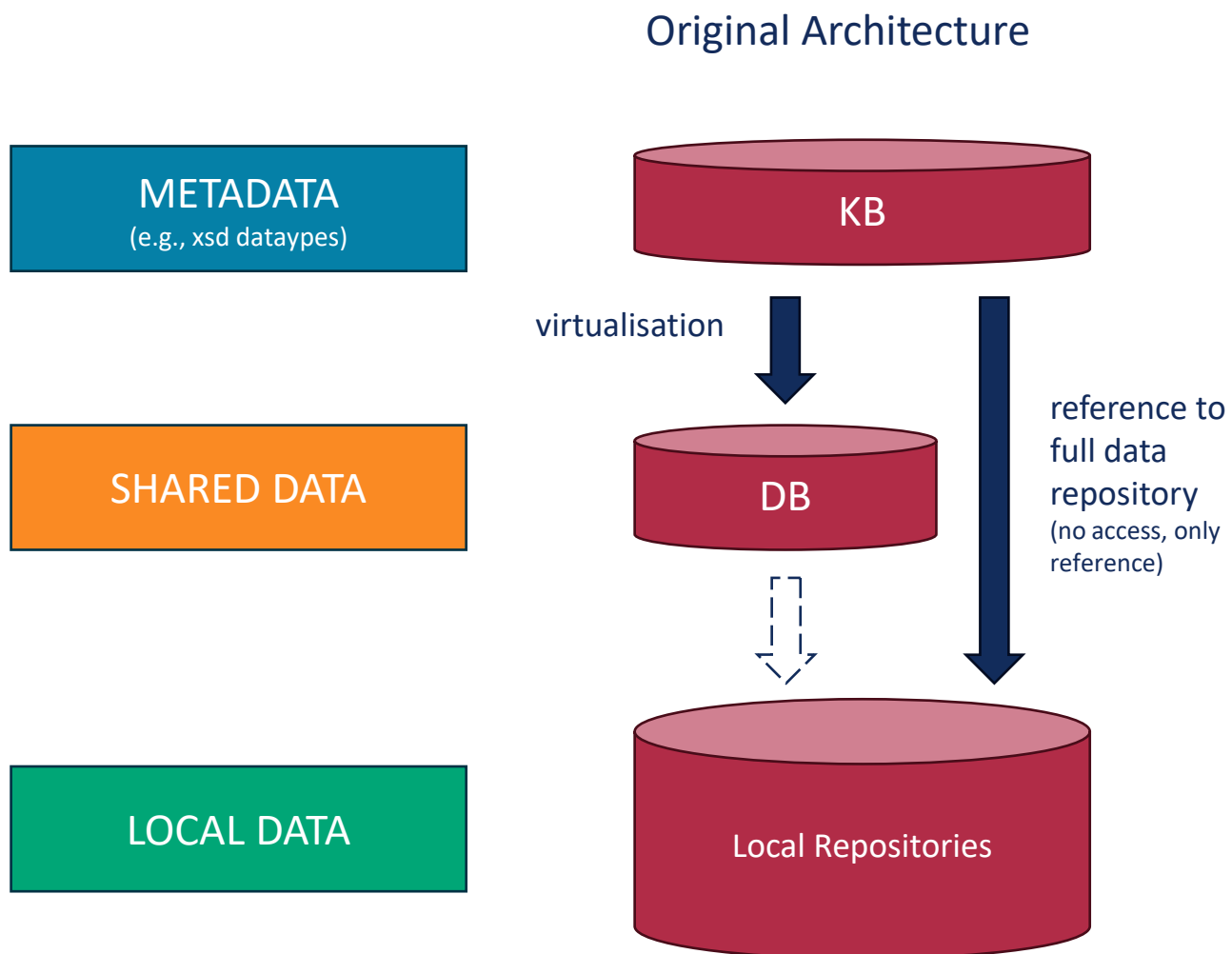
Field	Description
Sample ID	String: Sample name and identification number of test.
Measurement file	.mss, located in UNIROMA3's servers, contains all the information related to the measurement, and the complete raw results.
Indentation map	.PNG, located in UNIROMA3's servers, contains pictures of the indentation maps, (i.e. applied load [mN] vs penetration depth [nm] ).
Indentation Data	.dat, located in UNIROMA3's servers, contains all data from raw to final to obtain 3D map (i.e. applied load [mN] vs penetration depth [nm] ).

non  
RDFS



# 1. Planning

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## SHARED DATA and METADATA

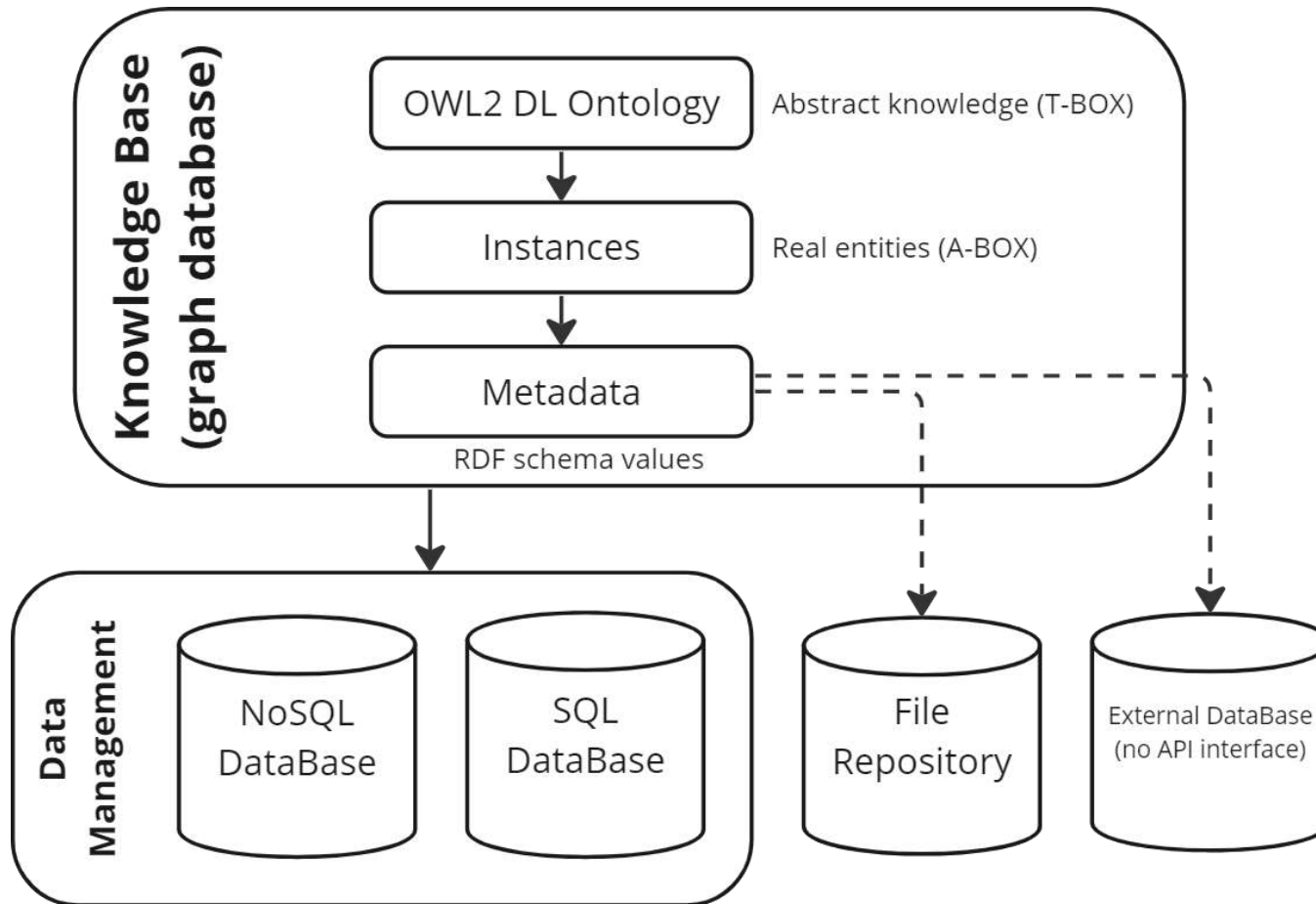
Field	Description
Sample ID	String: Sample name and identification number of test.
Sample description	String: sample composition and production information.
Test definition	String: Type of test and instrument name (i.e. Nanoindentation-Pillar splitting, MTS G200).
SOP file name	String: indication of the file name containing parameters of measurement (i.e. acquisition rate, max load, loading rate, approach speed etc.) .
Measurement Date Time	dd/mm/yyyy hh:mm:ss
Indenter	String: type of the indenter (i.e. Berkovich); serial number; material of the indenter.
Curves	Indentation curve: Load applied [N] vs penetration depth [m].
$P_c$	<b>mN</b> , the value of the critical load, identified from Indentation curve: (Load applied [N] vs penetration depth).
$K_{IC}$	<b>MPa<math>\sqrt{m}</math></b> , the value of the fracture toughness calculated from the value of the critical load.

## LOCAL DATA

Field	Description
Sample ID	String: Sample name and identification number of test.
Measurement file	<b>.mss</b> , located in UNIROMA3's servers, contains all the information related to the measurement and the complete results.
Indentation Data	<b>.xls</b> , located in UNIROMA3's servers, contains data, exported from .mss, needed for fracture toughness calculation (i.e. applied load [mN] vs penetration depth [nm]).

# 1. Planning

- o Did they plan a priori which data they needed, and how to extract knowledge from it?
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**Data Federation** is possible i.e. data can be made **directly reachable** from the KB through mapping with the graph database vendor querying system.

Data are **not directly reachable** from the KB but provide users with information about their location and accessibility.

## OTE Capabilities

(from OntoTrans and EMMC)

1. **Representing** manufacturing process challenges in a standard ontological form as technical and business Innovation Cases
2. **Connecting** innovation cases with existing appropriate information sources i.e. available data and materials modelling solutions
3. **Recommending** consistent materials modelling workflow options
4. **Supporting** simulation and validation activities
5. **Providing** semantic results interpretation to facilitate sharing and re-use of innovation cases and results



# 1. Planning

o Did they look for existing semantic assets to prepare for interoperability?

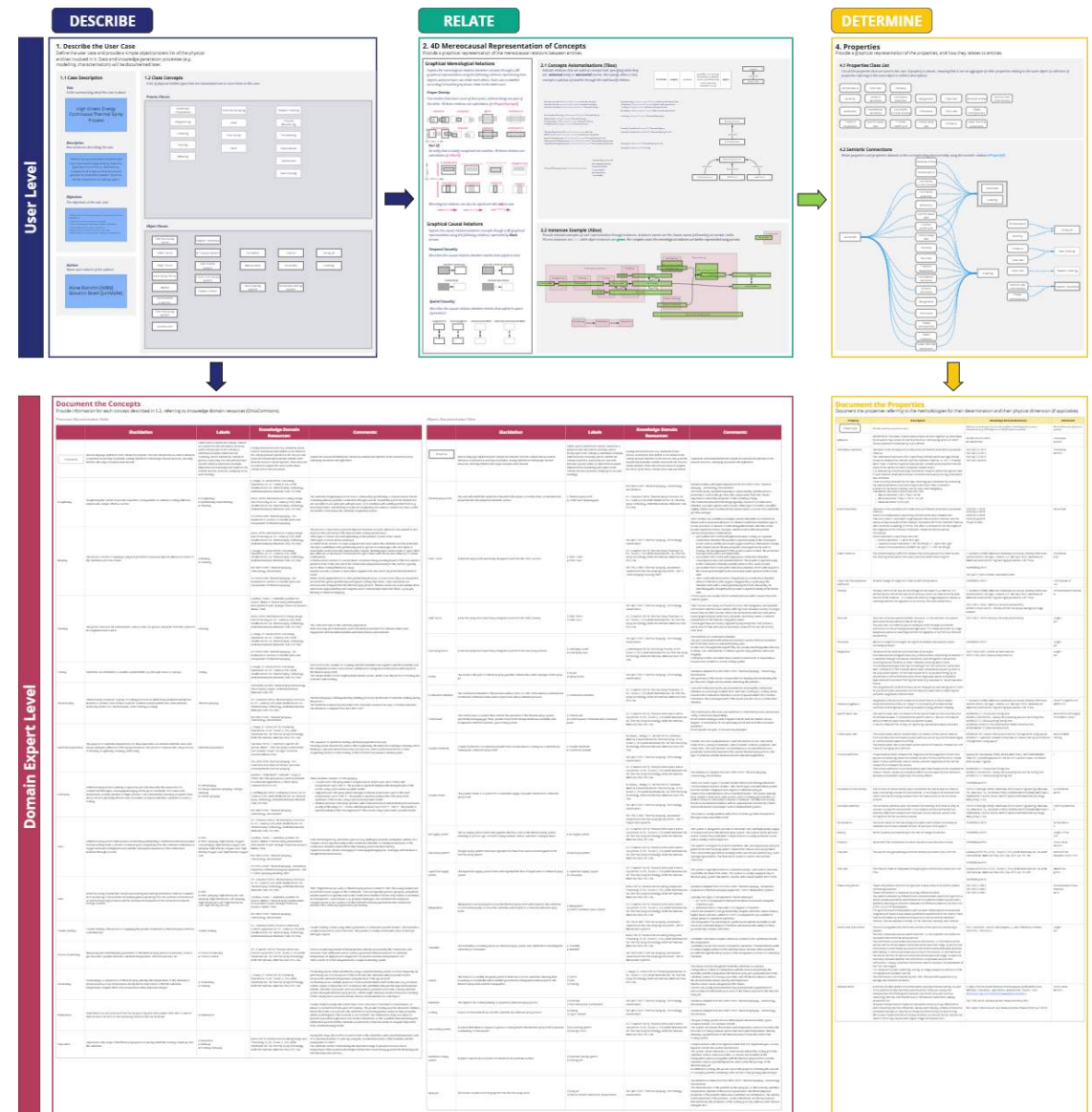


How to **extract the knowledge from domain experts** for an ontologist to create a formal representation of the domain knowledge (T-BOX of a **Domain Ontology**)?

## OntoTrans Conceptualisation Template!

Gathering and formalising a domain knowledge is done through the process of **conceptualisation**, i.e., by identifying ontological concepts in the form of **classes**, **relations**, and **axiomatic constraints** that cover the domain of interest.

To overcome the **barriers** coming from the **lack of expertise** in ontology engineering, the **OntoTrans project** has developed a methodology for the interaction between the **translator** and the industrial stakeholders, aimed to facilitate collective contributions to the conceptualization effort.





# 1. Planning

o Did they look for existing semantic assets to prepare for interoperability?



## DESCRIBE

### 1. Describe the User Case

Define the user case and provide a simple object/process list of the physical entities involved in it. Data and knowledge generation processes (e.g. modelling, characterisation) will be documented later.

#### 1.1 Case Description

**Title**  
A title summarizing what this case is about.

**High Kinetic Energy  
Continuous Thermal Spray  
Process**

**Description**  
Few sentences describing the case.

Thermal spray processes characterized by a high kinetic energy flow of a gas-powder mixture, obtained by expansion of a high pressure gas in a nozzle and by subsequent powder injection, for the deposition of coating layers.

**Objectives**  
The objectives of the user case.

Validation of process settings for high kinetic energy deposition.  
Validation of process parameters for high kinetic energy deposition.  
Validation of process parameters for high kinetic energy deposition.  
Validation of process parameters for high kinetic energy deposition.

**Authors**  
Name and contact of the authors.

Alvise Bianchini [MBN]  
Giovanni Rolli [UniMoRe]

#### 1.2 Class Concepts

A list of physical entities types that are instantiated one or more times in this case.

##### Process Classes



##### Object Classes



## RELATE

### 2. 4D Mereocausal Representation of Concepts

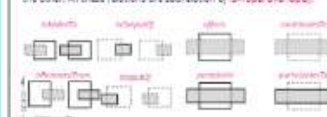
Provide a graphical representation of the mereocausal relations between entities.

#### Graphical Mereological Relations

Express the mereological relations between concepts through a 4D graphical representation using the following schemes, representing how objects and processes can relate with others. Each case is labelled according to how the gray boxes relate to the white ones.

##### Proper Overlap

Two entities that share some of their parts, without being one part of the other. All these relations are subtypes of *isProperOverlapOf*.



##### Part of

An entity that is totally comprised into another. All these relations are subtypes of *isPartOf*.



Mereological relations can also be expressed with red arrows.

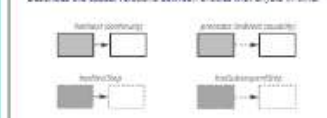


#### Graphical Causal Relations

Express the causal relations between concepts through a 4D graphical representation using the following relations, expressed by black arrows.

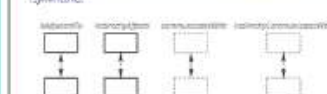
##### Temporal Causality

Describes the causal relations between entities that unfold in time.



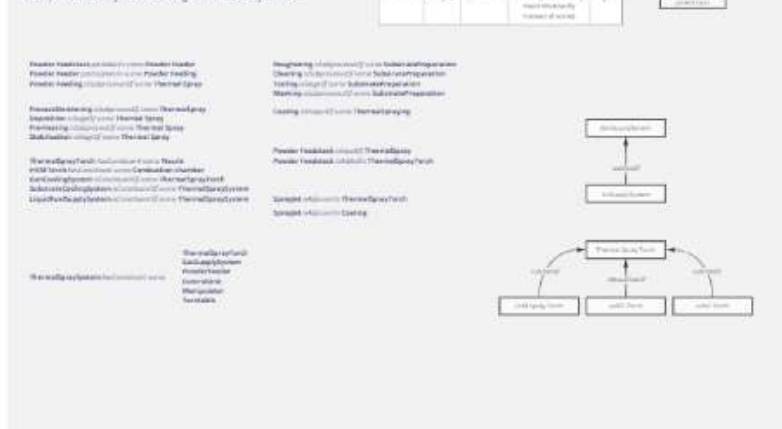
##### Spatial Causality

Describes the causal relations between entities that unfold in space (symmetrical).



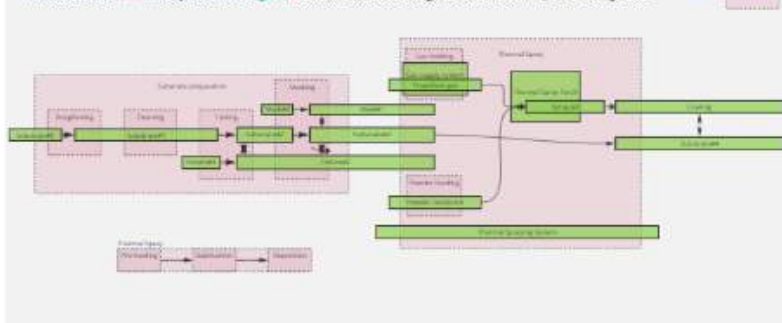
#### 2.1 Concepts Axiomatisations (TBox)

Indicate relations that are valid at concept level, specifying when they are *universal* (only) or *existential* (some). Also specify when a class concept is a subclass of another through the *subClassOf* relation.



#### 2.2 Instances Example (ABox)

Provide relevant examples of class representation through instances. Instance names are the classes names followed by an number index. Process instances are *pink* while object instances are *green*. For complete cases the mereological relations are better represented using arrows.

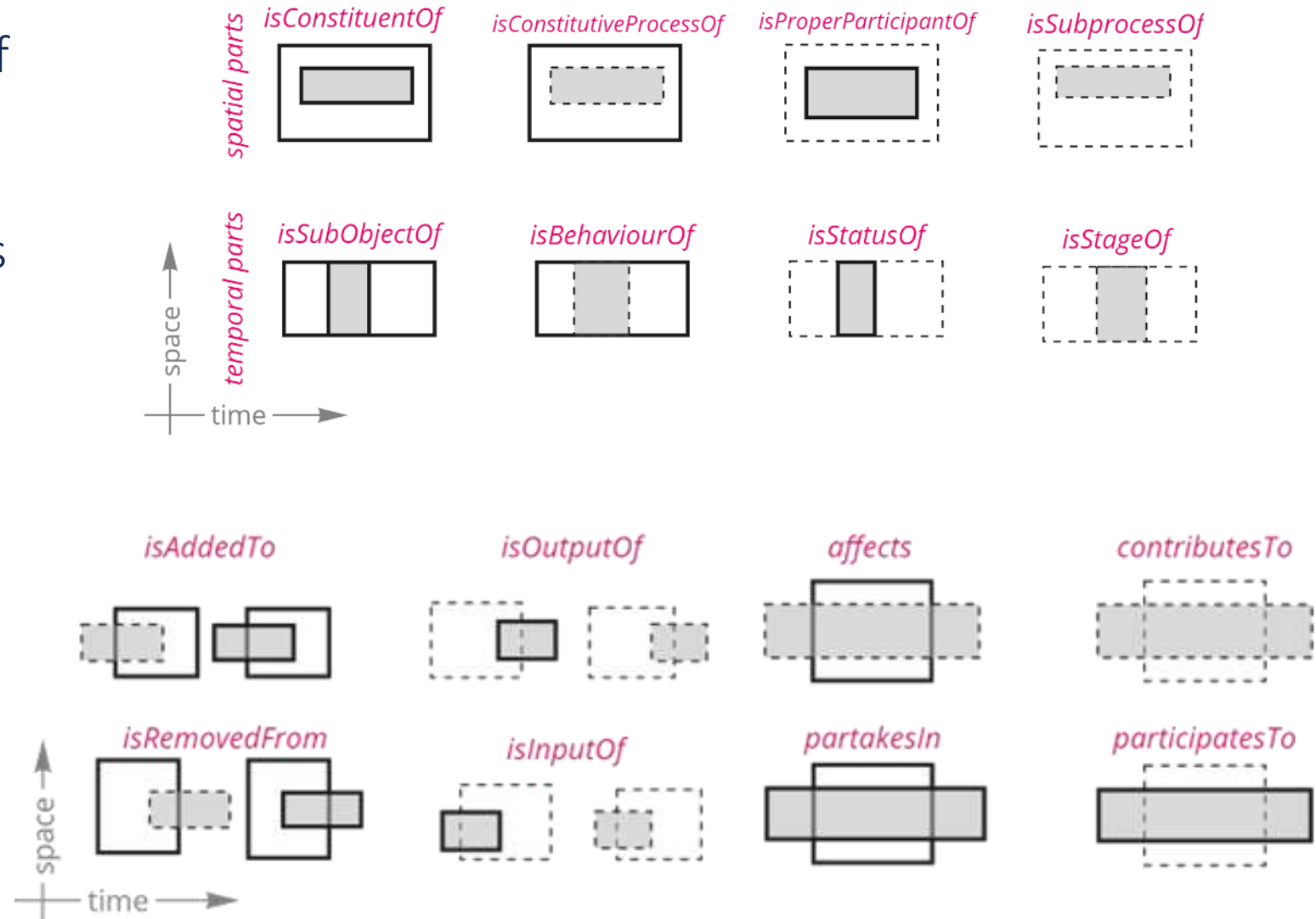


# 1. Planning

o Did they look for existing semantic assets to prepare for interoperability?



A simple visual summary of EMMO fundamental ontological relations has been provided to the users to let them understand how an ontology formalise the relations between entities.

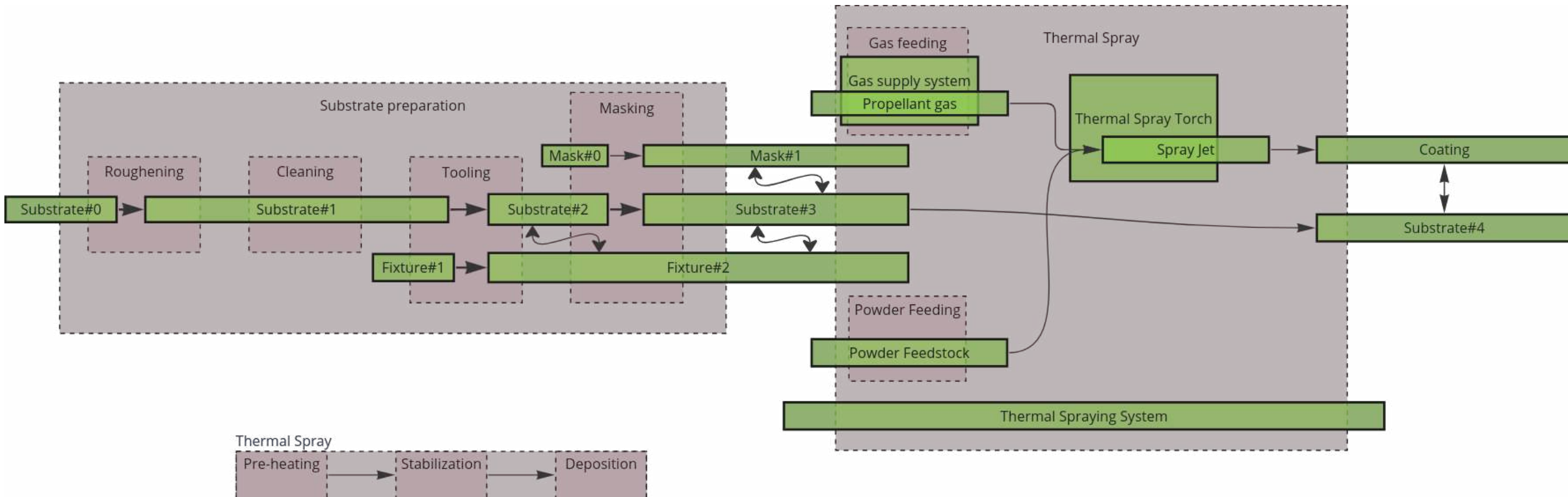


# 1. Planning

o Did they look for existing semantic assets to prepare for interoperability?



4D conceptual representation of a Thermal Spraying process, connecting all the relevant entities using EMMO mereocausality relations, to document the **overall state of things**.



# 1. Planning

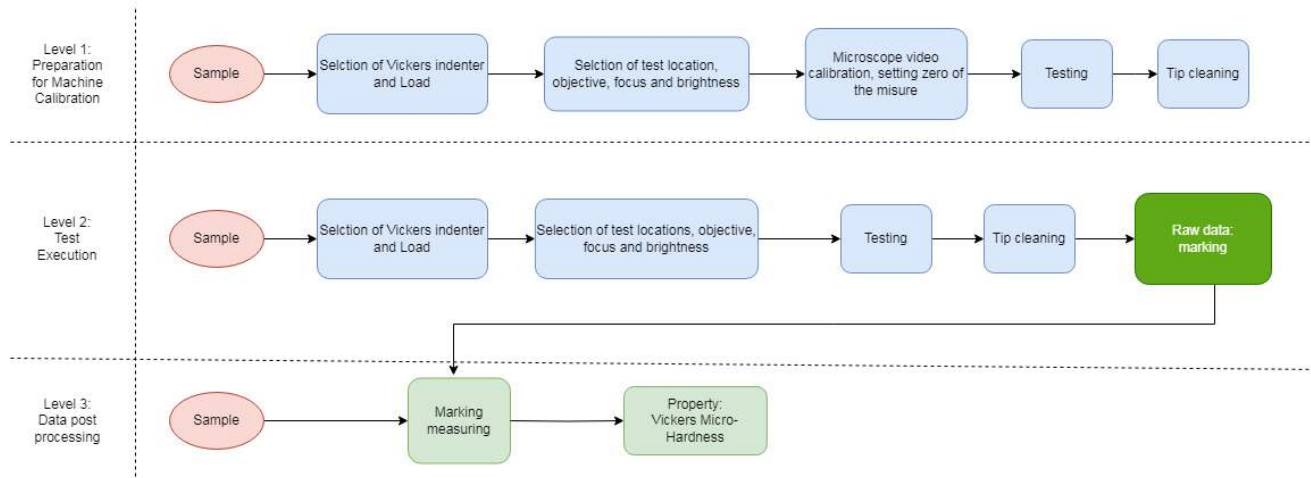
o Did they look for existing semantic assets to prepare for interoperability?



MODA and CHADA templates have been used mainly to document modelling and characterisation workflows.

Their ontological representation has been simplified since we had to focus more on data mapping and ingestion.

Vickers Micro-Hardness



4. DATA PROCESSING		
4.1	Level of expertise	Little expertise: Person can read out results directly
	Data normalisation	None
3. RAW DATA		
3.1	Raw Data	Vickers tip residual imprint
3.2	Unit	X coordinate - $\mu m$ Y coordinate - $\mu m$
2. EXPERIMENT		
Interaction nature and character (destructive or non-destructive) of the probe with the sample		
	Probe/Physics of	<ul style="list-style-type: none"> <li>Elastic Deformation: As the diamond indenter contacts the material's surface, it exerts a force, causing elastic deformation in both the diamond indenter and the material. Elastic deformation occurs when the atoms in the material are displaced from their equilibrium positions but return to their original positions once the force is removed.</li> </ul>
1. USER CASE		
1.1	USER	The user must be properly trained in the execution of the experiment, including the simple manual operations that need to be performed with accuracy.
1.2	User case (sample)	No specific Sample dimensions is required for the test, however, it is and polished.
OVERVIEW OF THE CHARACTERISATION		
1	User Case	Any solid sample can be tested included bulk material, coating, heterogeneous material, biomaterial and no specific Sample dimensions is required. Environment: Laboratory air, room temperature.
2	Characterisation method	<p>Hardness Value Determination. Additionally, the Vickers microhardness test can be combined with other characterization techniques to gain further insights into the material's properties:</p> <ul style="list-style-type: none"> <li>combined with microstructural analysis using microscopy techniques can provide a correlation between the material's microstructure and its hardness properties;</li> <li>Phase Identification is possible identifying variations in hardness;</li> <li>Depth Profiling, combined with indentation depth measurements to assess the hardness as a function of depth below the sample surface.</li> </ul>
3	Validation of Characterisation	Vickers microhardness not only provides information about the hardness, but can also be used to assess other mechanical properties such as cohesion, and adhesion of the coating to the substrate. Hardness measurement can be correlated with other coating properties and help evaluate its suitability for specific applications.
4	Access conditions (what is needed to repeat the experiment)	<p>The sample preparation requires an in-house routine.</p> <p>The characterisation tool requires an in-house routine.</p>



- o Did they look for existing semantic assets to prepare for interoperability?



cobrain (http://emmo.info/emmo/cobrain) : [/home/emanuele/Desktop/cobrain.ttl]

File Edit View Reasoner Tools Refactor Window Help

< > cobrain (http://emmo.info/emmo/cobrain)

Object ThermalSpraySystem

Active ontology x Entities x Individuals by class x DL Query x Individual Hierarchy Tab x

Annotation properties Datatypes Individuals

Classes Object properties Data properties

Class hierarchy: ThermalSpraySystem

Annotations

Annotations: ThermalSpraySystem

Annotations

skos:prefLabel [language: en]  
ThermalSpraySystem

Description: ThermalSpraySystem

Equivalent To

SubClass Of

inverse (isConstituentOf) some ControlUnit  
inverse (isConstituentOf) some GasSupplySystem  
inverse (isConstituentOf) some Manipulator  
inverse (isConstituentOf) some PowderFeeder  
inverse (isConstituentOf) some ThermalSprayTorch  
inverse (isConstituentOf) some Turntable  
Object

General class axioms

SubClass Of (Anonymous Ancestor)

Instances

Target for Key

Rules:

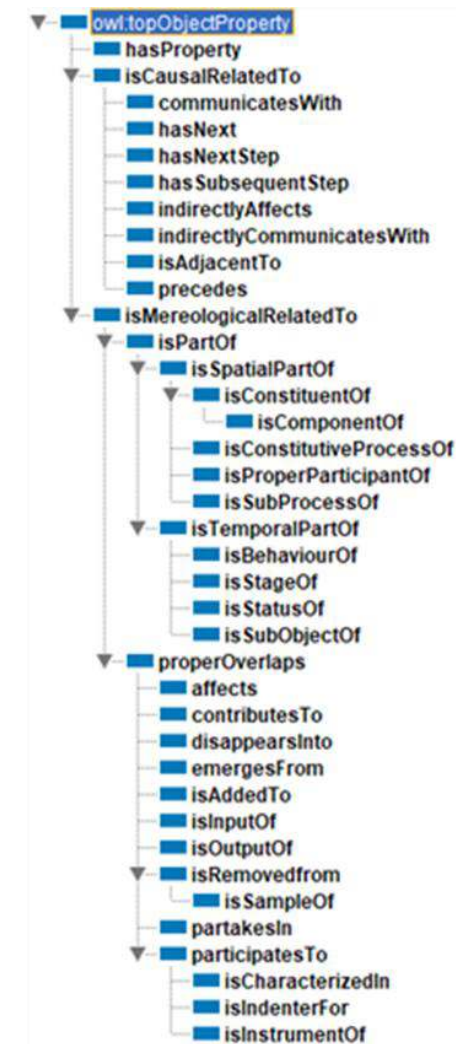
Rules

OWL Viz: ThermalSpraySystem

Asserted hierarchy Inferred hierarchy

```

graph TD
    owlThing[owl:Thing] --> Object[Object]
    Object --> SupplySystem[SupplySystem]
    Object --> ThermalSprayTorch[ThermalSprayTorch]
    SupplySystem --> LiquidFuelSupplySystem[LiquidFuelSupplySystem]
    SupplySystem --> AirSupplySystem[AirSupplySystem]
    GasSupplySystem[GasSupplySystem] --> AirSupplySystem
    ThermalSprayTorch --> PlasmaSprayTorch[PlasmaSprayTorch]
    ThermalSprayTorch --> HVOFTorch[HVOFTorch]
    ThermalSprayTorch --> ColdSprayTorch[ColdSprayTorch]
    ThermalSprayTorch --> HVAFTorch[HVAFTorch]
  
```

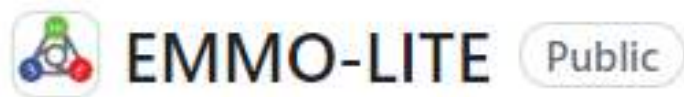


# 1. Planning

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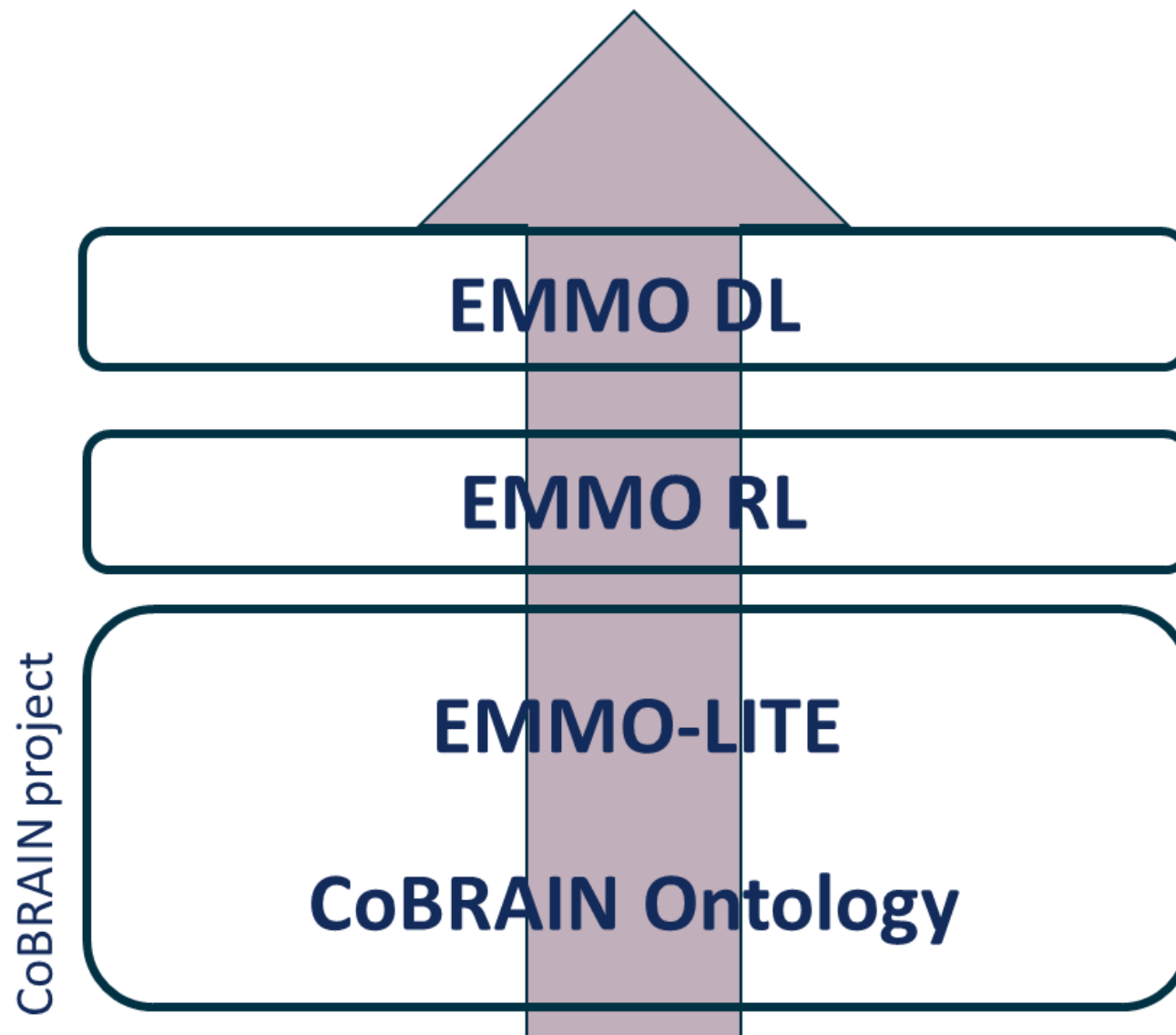
EMMO-LITE has been used as a reference ontology, to **facilitate** usage by non-EMMO experts



<https://github.com/emmo-repo/EMMO-LITE>



<https://github.com/cobrain-project/ontology>



# 1. Planning

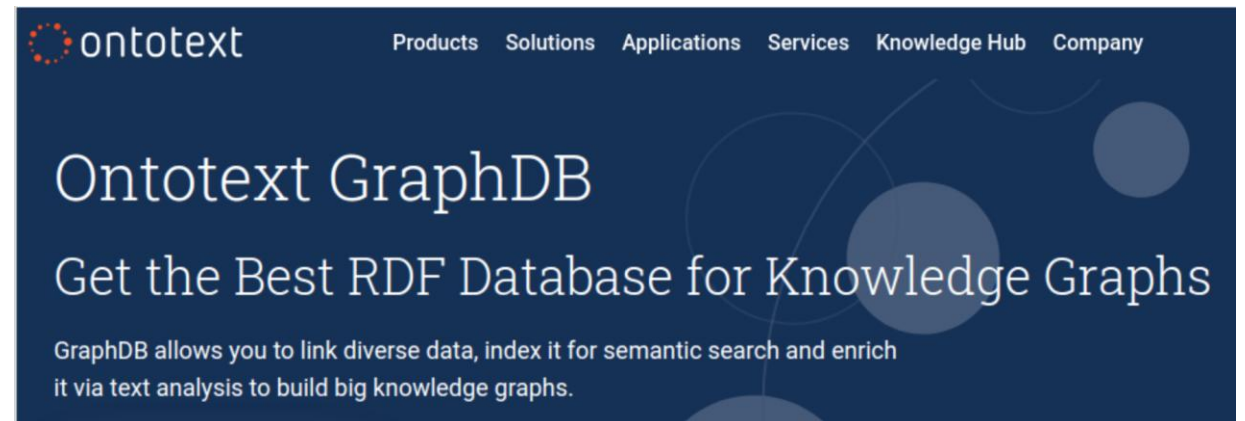
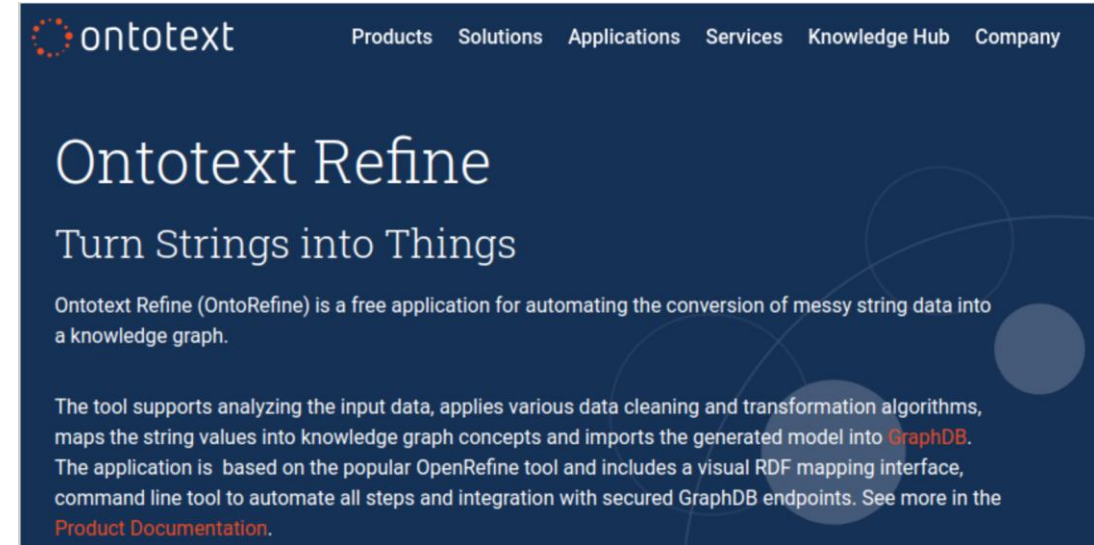
o Did they purchase software and or equipment to produce data?



Key point for the CoBRAIN Knowledge Management Platform design:

**No wheel reinventing!**

The overall system must rely on existing commercial tools with free-to-use licensing option and W3C standards that have reached a significant level of maturity.

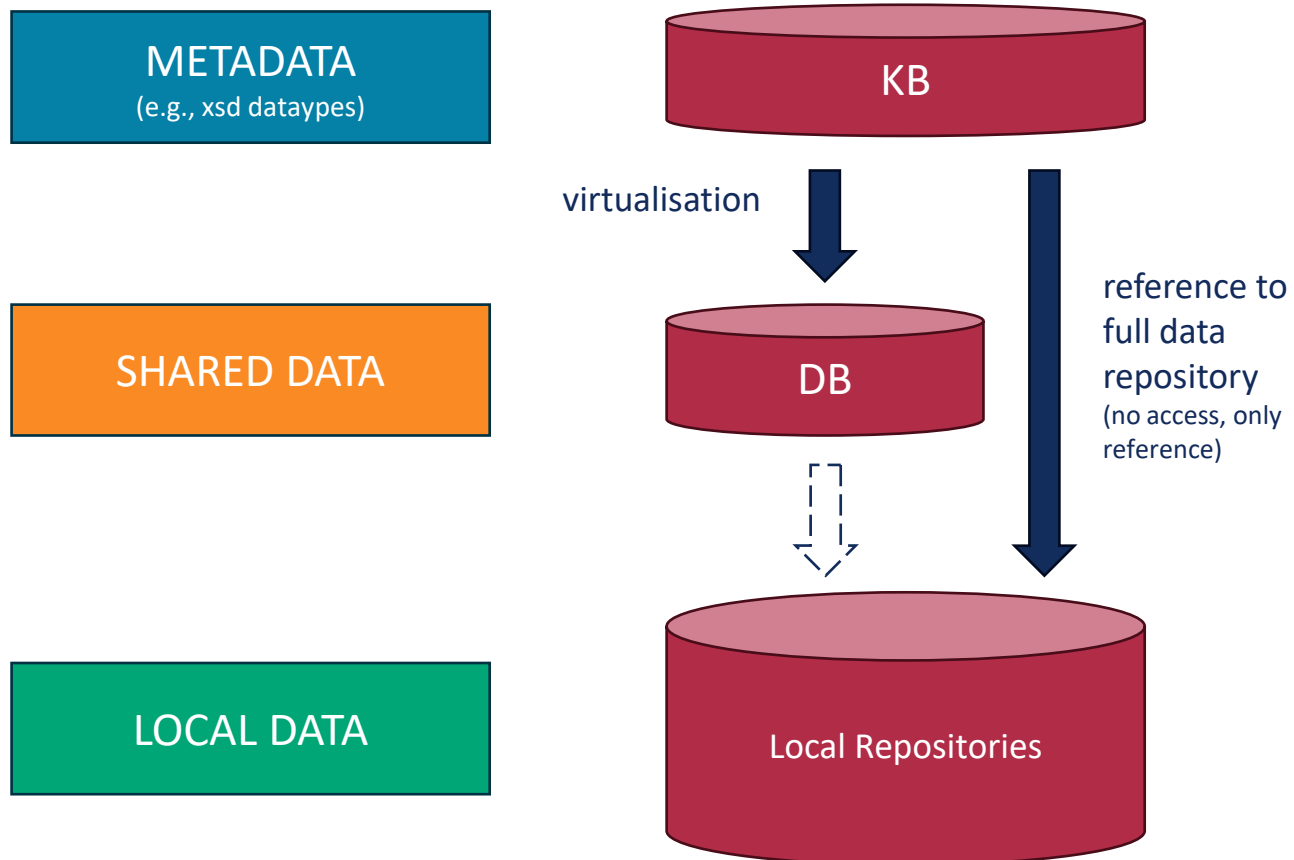


## 2. Acquiring

- o How is data acquired?
- o Are meta data acquired?



### Original Architecture



### SHARED DATA and METADATA

Field	Description
Sample ID	String: Sample name and identification number of test.
Sample description	String: sample composition and production information.
Test definition	String: Type of test and instrument name (i.e. Nanoindentation-Pillar splitting, MTS G200).
SOP file name	String: indication of the file name containing parameters of measurement (i.e. acquisition rate, max load, loading rate, approach speed etc.) .
Measurement Date Time	dd/mm/yyyy hh:mm:ss
Indenter	String: type of the indenter (i.e. Berkovich); serial number; material of the indenter.
Curves	Indentation curve: Load applied [N] vs penetration depth [m].
$P_c$	<b>mN</b> , the value of the critical load, identified from Indentation curve: (Load applied [N] vs penetration depth).
$K_{IC}$	<b>MPa√m</b> , the value of the fracture toughness calculated from the value of the critical load.

### LOCAL DATA

Field	Description
Sample ID	String: Sample name and identification number of test.
Measurement file	<b>.mss</b> , located in UNIROMA3's servers, contains all the information related to the measurement and the complete results.
Indentation Data	<b>.xls</b> , located in UNIROMA3's servers, contains data, exported from .mss, needed for fracture toughness calculation (i.e. applied load [mN] vs penetration depth [nm]).



## 2. Acquiring

- o How is data acquired?
- o Are meta data acquired?



### METADATA

(stored in KB as e.g., xsd datatypes)

### SHARED DATA

(stored in KB as e.g., xsd datatypes)

#### SHARED DATA and METADATA

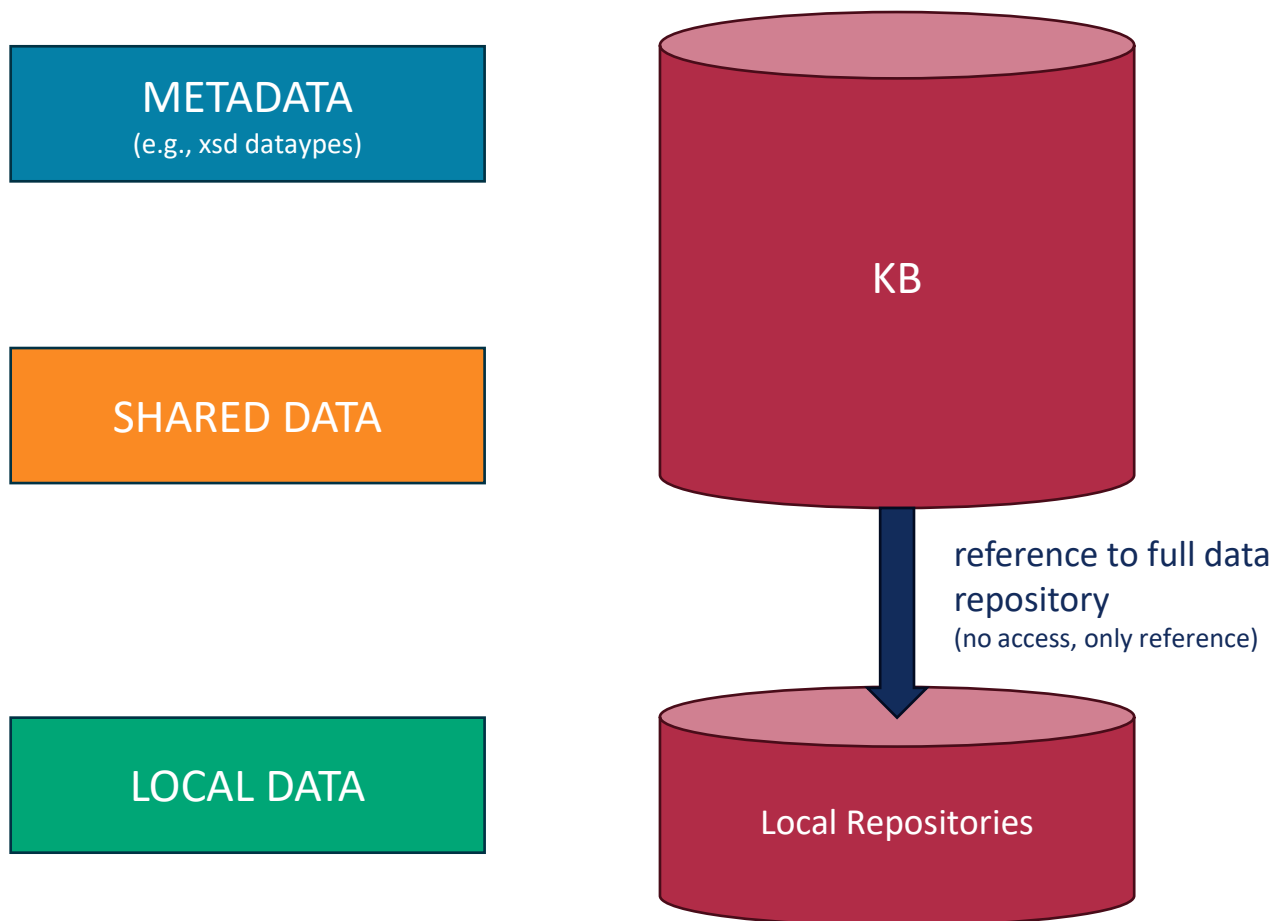
Field	Description
Measurement type	<b>String:</b> "Volume di una buca o un picco:" followed by a shortened form of the string indicating the name of the original file and the elaboration operation
File name	<b>String:</b> Original profilometer file including path
Date/time	<b>yyyy/mm/dd hh:mm:ss:</b> date and time of elaboration
Hole surface	<b>μm<sup>2</sup>:</b> area of the projected surface occupied by peaks, followed by a string listing the complete sequence of operations leading to the elaborated profile
Peak surface	<b>μm<sup>2</sup>:</b> area of the projected surface occupied by peaks, followed by a string listing the complete sequence of operations leading to the elaborated profile
Hole volume	<b>μm<sup>3</sup>:</b> overall volume of the hole (below the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Peak volume	<b>μm<sup>3</sup>:</b> overall volume of the peaks (above the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Maximum depth (hole)	<b>μm:</b> maximum depth of the hole (below the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Maximum height (peak)	<b>μm:</b> maximum height of the hole (below the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Average depth (hole)	<b>μm:</b> average depth of the hole (below the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Average height (peak)	<b>μm:</b> average height of the hole (below the reference plane), followed by a string listing the complete sequence of operations leading to the elaborated profile
Objective	<b>String:</b> Magnification of the objective employed in the measurement [optional, user-typed, inserted in the first measurement file]
Step	<b>μm:</b> z-scan step size [optional, user-typed, inserted in the first measurement file]

## 2. Acquiring

- o How is data acquired?
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Unfortunately, local data management in the form of local query-able databases (e.g., MongoDB, SQL) as foreseen in the GA was not a realistic possibility for partners... so we dropped virtualisation



### SHARED DATA and METADATA

Field	Description
Sample ID	String: Sample name and identification number of test.
Sample description	String: sample composition and production information.
Test definition	String: Type of test and instrument name (i.e. Nanoindentation-Pillar splitting, MTS G200).
SOP file name	String: indication of the file name containing parameters of measurement (i.e. acquisition rate, max load, loading rate, approach speed etc.) .
Measurement Date Time	dd/mm/aaaa hh:mm:ss
Indenters	String: type of the indenter (i.e. Berkovich); serial number; material of the indenter.
Curves	Indentation curve: Load applied [N] vs penetration depth [m].
$P_c$	<b>mN</b> , the value of the critical load, identified from Indentation curve: (Load applied [N] vs penetration depth).
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- o How is data acquired?
- o Are meta data acquired?



Data are acquired and **stored locally** using **partner's specific methods and formats**.

Most of them are **Excel tables**. Some data are in **JSON format** (unfortunately not JSON-LD).

### Example of tabular data providing HVOF process details.

Sample ID	Nominal Composition	Lot. N.	Substrate	Date	Run n°	length mm	width mm	FR H <sub>2</sub> FMR	p H <sub>2</sub> psi	FR O <sub>2</sub> psi	p O <sub>2</sub> psi	FR / p Air FM psi	Pwdr. Feed g/min	Standoff mm	Pitch mm	Speed mm/s	n° cycles	e	passes	weight in g	weight fin g	weight in g	weight fin g	weight in g	weight fin g	gain g	sprayed mass g	efficiency	
AlO(CrMnFeNi)+60TiC RUN1	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	1	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN2	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	2	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN3	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	3	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN4	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	4	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN5	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	5	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN6	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	6	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN7	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	7	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN8	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	8	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN9	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	9	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN10	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	10	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN11	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	11	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN12	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	12	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN13	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	13	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN14	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	14	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN15	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	15	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN16	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	16	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN17	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	17	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN18	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	18	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN19	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	19	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN20	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	20	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN21	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	21	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN22	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	22	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN23	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	23	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN24	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	24	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN25	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	25	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN26	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	26	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN27	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	27	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN28	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	28	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN29	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	29	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN30	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	30	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN31	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	31	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN32	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	32	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN33	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	33	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN34	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	34	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN35	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	35	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN36	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	36	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN37	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	37	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN38	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	38	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN39	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	39	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN40	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	40	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN41	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	41	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34,67	37,76	34,35	37,5	34,26	37,35	3,11	5,2	59,8
AlO(CrMnFeNi)+60TiC RUN42	AlO(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	19/02/2024	4																								

## 2. Acquiring

- o How is data acquired?
- o Are meta data acquired?



**Ideal solution:** a new project that implements a **full framework for assisted/automated data collection** for all CoBRAIN datasets, providing a built-in semantic enhancement of data

**Proposed Solution:** UNIBO will **refactor all collected data**, providing as-much-as-possible **constrained templates** for data collection (“if you can't beat them, join them”)

METADATA											DATA			
Sample				Test					Indenter					
Sample ID	Composition	Production Information	Origin ID	Test ID	Test Type	Instrument ID	SOP File	DateTime	Type	S/N	Material	Indentation Curve	Pc	KIC
FC00q8	[[Cu,Zn],[65,35]]	Some text about sample production	yQvzd7	h2baA2	PillarSplitting	MTSG200-1	<a href="file://emanuele@kant.unibo.it:22/home/emanuele/file3.txt">file://emanuele@kant.unibo.it:22/home/emanuele/file3.txt</a>	12/3/2023 11:54	Berkovich	XIUQ32	W	[[1,2,3],[1,2,3]]	12	34
TatORe	[[Cu,65],[Zn,35]]	Some other text about sample production	yQvzd7	ap6eUT	PillarSplitting	MTSG200-1	<a href="file://emanuele@kant.unibo.it:22/home/emanuele/file5.txt">file://emanuele@kant.unibo.it:22/home/emanuele/file5.txt</a>	14/3/2023 12:54:00 AM	Berkovich	XIUQ32	W	[[1,3,4],[2,1,5]]	5	3



- o What types of data are there?
- o Are the data described as and when they come in?

21

# 3. Processing

- o How are data extracted?
- o Are there automatic workflows in place?

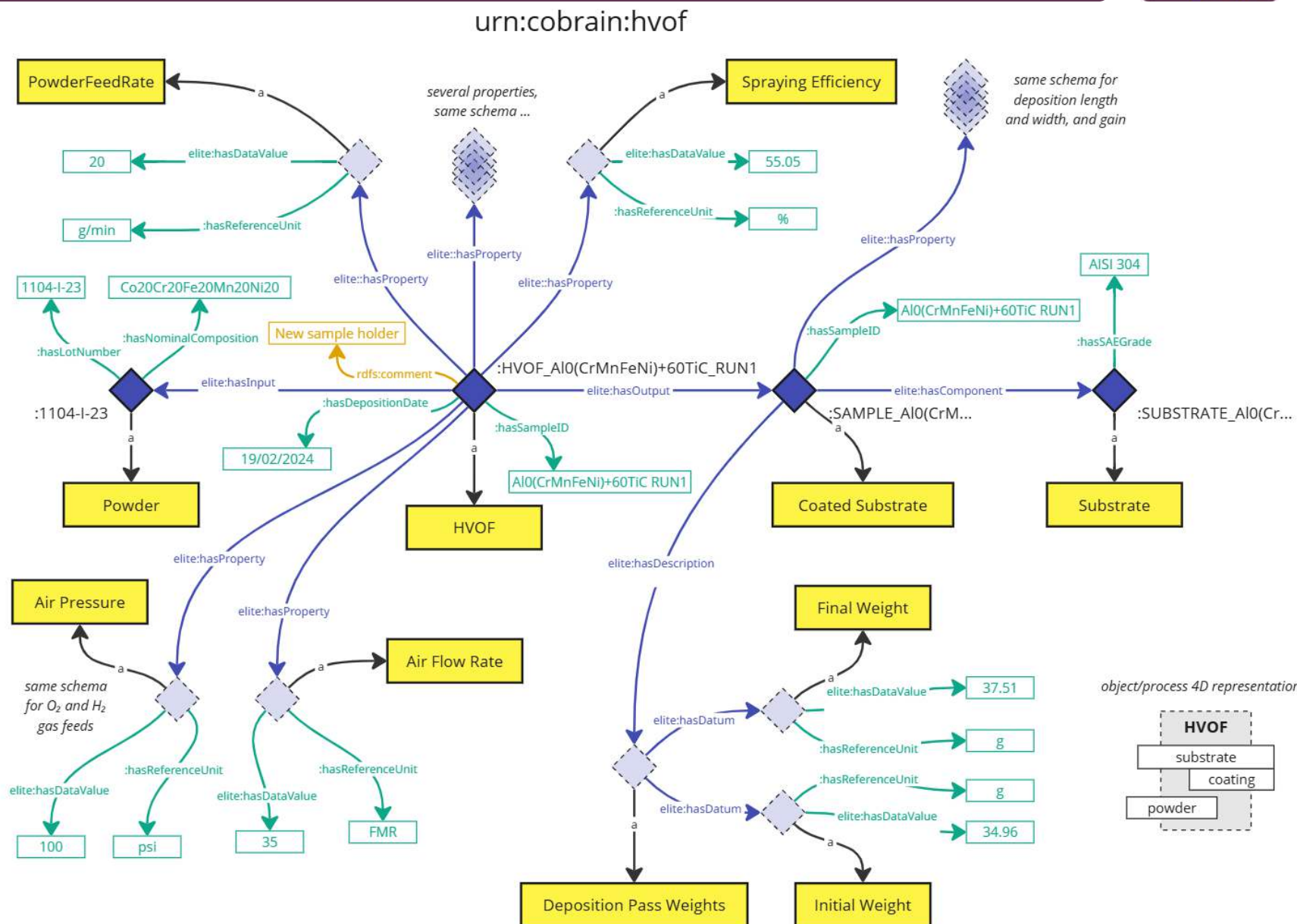
- o How is provenance ensured?



## Graphical Approach to Conceptual Mapping

Partners collaborated with UNIBO to build the conceptual mapping between the Excel file columns and the ontological concepts, including relations.

UMR HVOF Thermal Spraying Logbook



# 3. Processing

- o How are data extracted?
- o Are there automatic workflows in place?

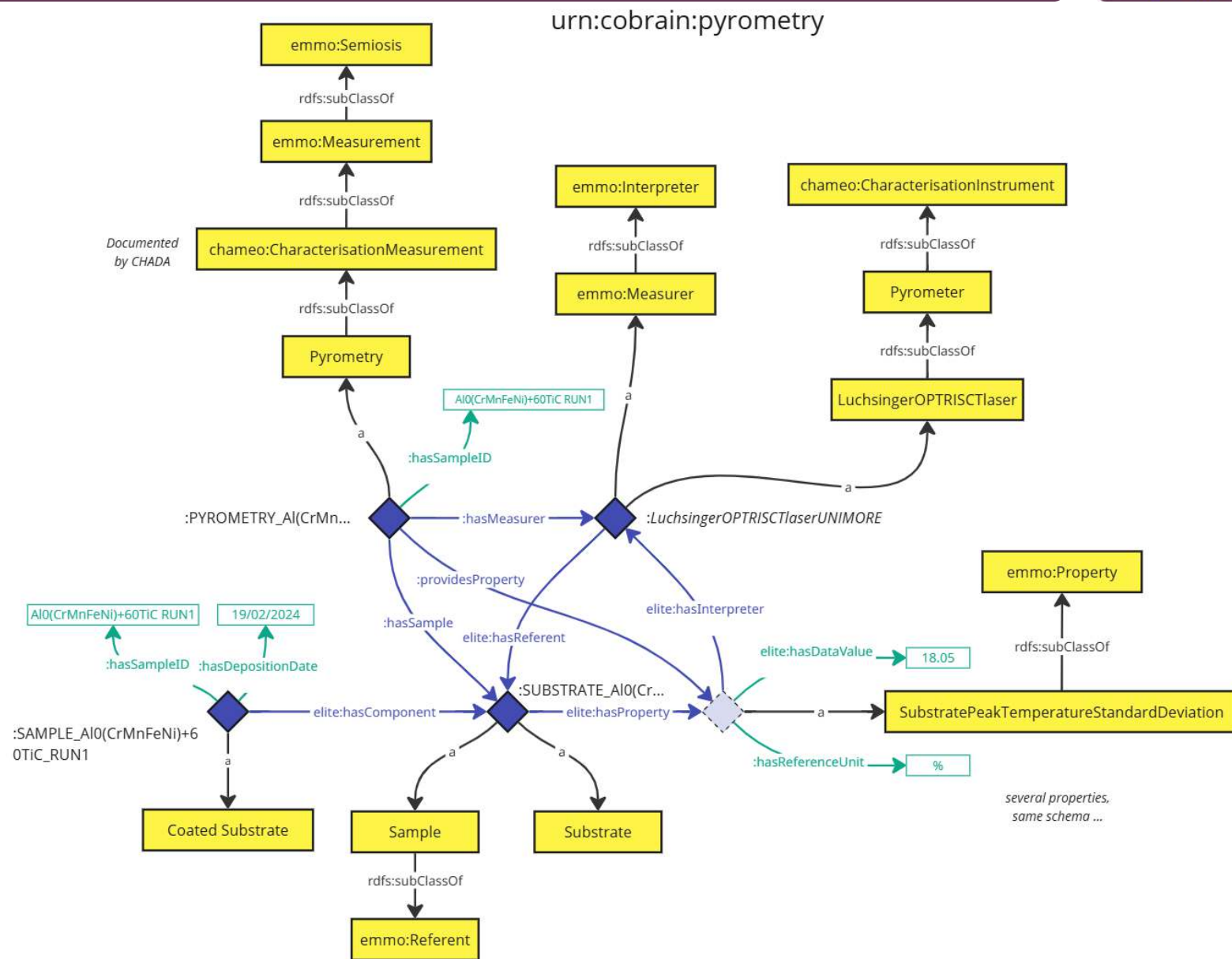
o How is provenance ensured?



## Graphical Approach to Conceptual Mapping

Partners collaborated with UNIBO to build the conceptual mapping between the Excel file columns and the ontological concepts, including relations.

Optical pyrometer Luchsinger OPTRIS CTlaser





# 3. Processing

- o How are data extracted?
- o Are there automatic workflows in place?

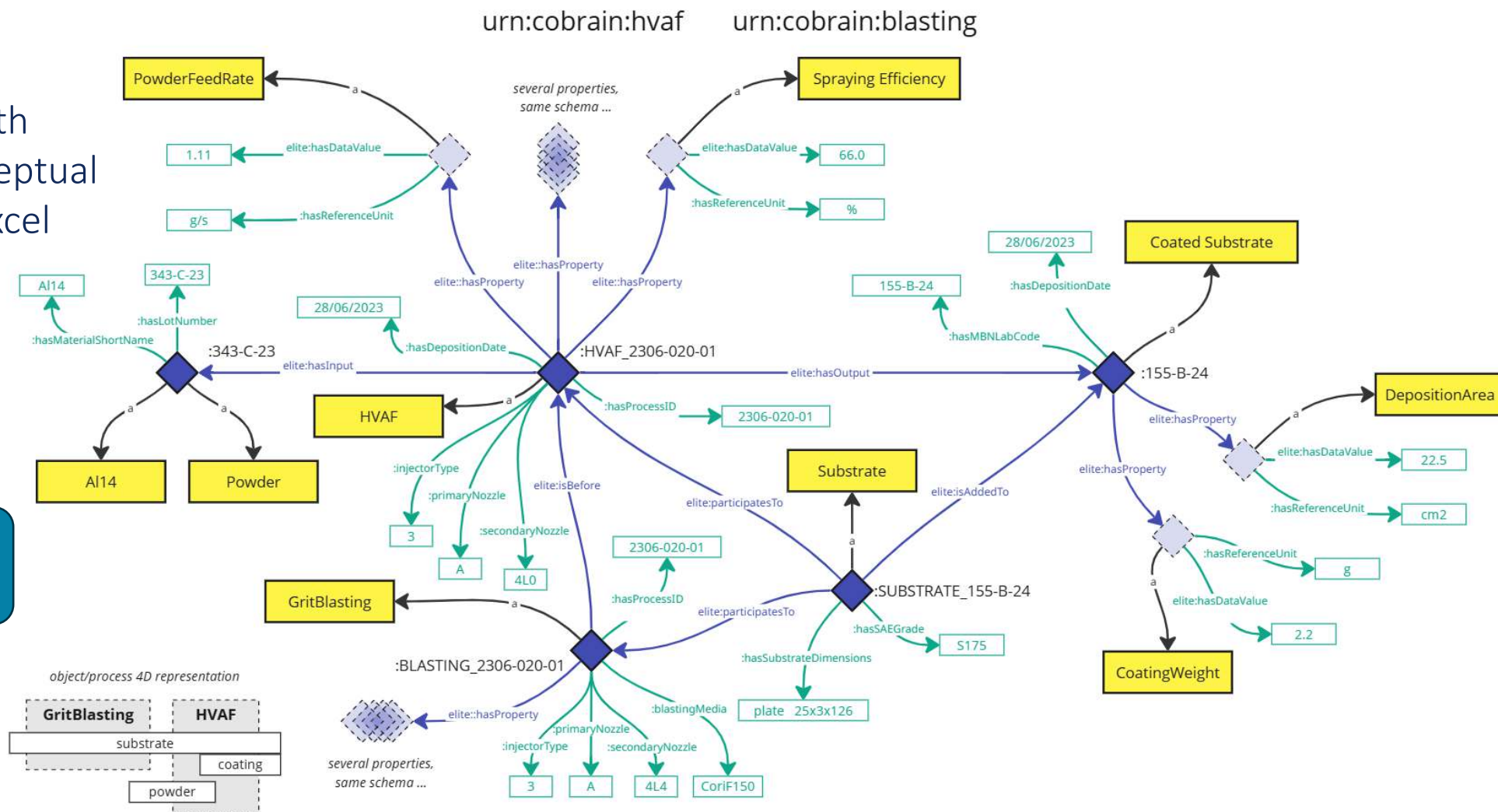
o How is provenance ensured?



## Graphical Approach to Conceptual Mapping

Partners collaborated with UNIBO to build the conceptual mapping between the Excel file columns and the ontological concepts, including relations.

HVAF Thermal Spraying Logbook + Grit Blasting



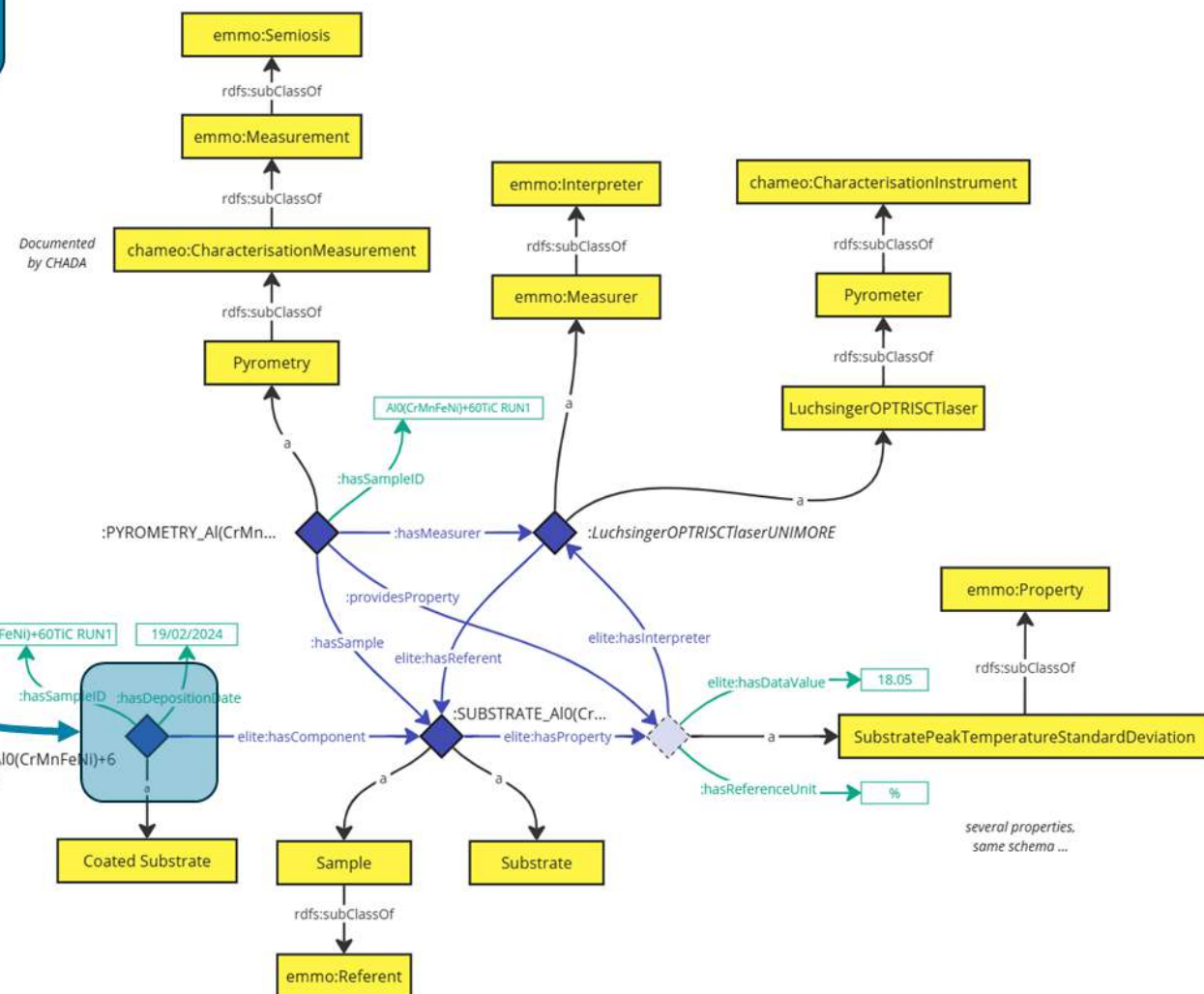


- o How are data extracted?
- o Are there automatic workflows in place?



Co-BRAIN

Optical pyrometer Luchsinger  
OPTRIS CTlaser



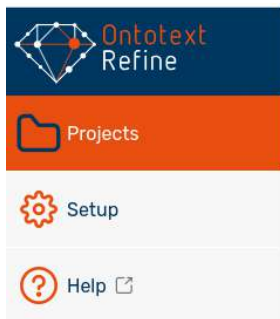
# 3. Processing

- o How are data extracted?
- o Are there automatic workflows in place?

- o How is provenance ensured?



## Mapping of HVOF Pyrometry UNIMORE T3.2 with OntoRefine



Name: AI0(CrMnFeNi) Run1 20230720 t... Identifier: 2392817068477

Visual RDF Mapper

SPARQL Query Editor

Configuration Preview Both

All mapping changes saved Save Download JSON Upload JSON RDF Open in GraphDB New Mapping

- Sample\_ID - D ... ymmdd - t ... \_unit - a ... axima - s ... axima - t ... peaks - @ ... - @id - @ ... @type

Base IRI  
http://example.com/base/

Use the current repository prefixes or add new using the Turtle or SPARQL syntax, i.e PREFIX rdf: <http://www.w3.org/1999/02/22-rdf-syntax-ns#>

cobrain elite xsd

cobrain: - Sample_ID	<IRI>	a	<IRI>	cobrain: CoatedSubstrate	<IRI>
		cobrain: hasDatetime	<IRI>	- Dep ... yyymmdd	"Literal"
				xsd: dateTime	^^Datatype
		elite: hasProperty	<IRI>	- Sample_ID	_:Unique BNode
		a	<IRI>	cobrain: Substra ... erature	<IRI>
		cobrain: hasReferenceUnit	<IRI>	- tem ... re_unit	"Literal"
				xsd: string	^^Datatype
		elite: hasDataValue	<IRI>	- ave ... _maxima	"Literal"
				xsd: float	^^Datatype

### 3. Processing

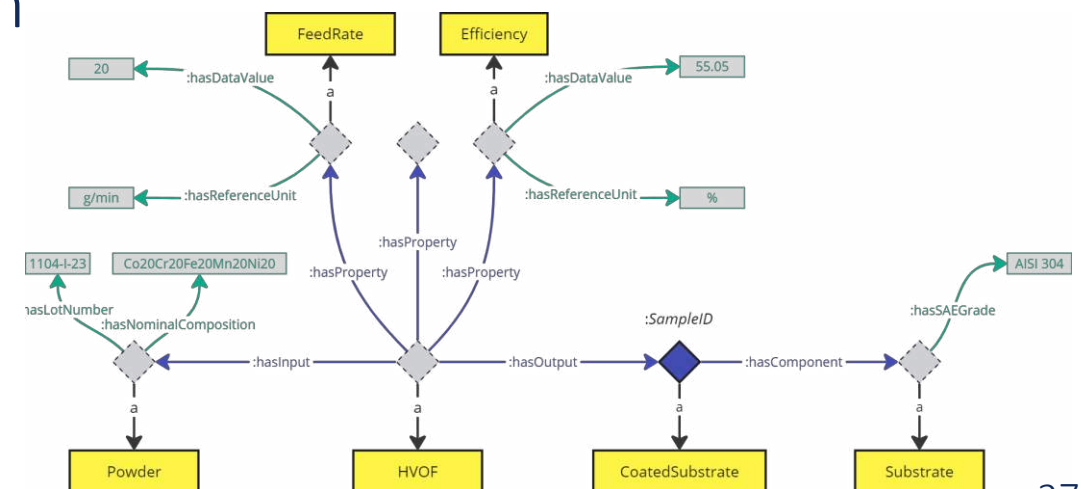
- o How are data extracted?
- o Are there automatic workflows in place?

- o How is provenance ensured?



We have found **some practical issues** in the excel-oriented approach experimental and characterisation datasets:

- **Unprecise IDs** (e.g., case change, spaces, use of reserved character)
- **Non-Unique IDs**: same ID used for e.g., deposition, sample, substrate...
- **Multiple intended interpretation for the same cell-value**, leading to an excessive blank-node rich representation
- **Too many degree of freedom** for the user to fill the sheets, leading to inconsistencies and scattered text



## 4. Analysing

What tools did/will your project develop to extract knowledge from your data?



SPARQL stands for SPARQL Protocol and RDF Query Language

SPARQL is a standard semantic query language for databases used for manipulating and retrieving data in the RDF (Resource Description Framework) format

RDF is a data model for representing information as a set of triples.

A triple consists of a subject, predicate, and object:

- **Subject:** Represents a resource (e.g., a person, a place).
- **Predicate:** Describes a property or relationship of the subject.
- **Object:** The value of the property or the resource related to the subject.

Subjects and predicates are always URI identifiers, but objects can be URIs or literal values.



## 4. Analysing

What tools did/will your project develop to extract knowledge from your data?



```
PREFIX mov: <http://example.org/ontology/movies#>
```

Prefixes allow to substitute the full IRI with a concise version

```
SELECT DISTINCT ?movie ?genre WHERE {
```

Select the desired elements, in this case without duplicates

```
  ?movie mov:director mov:StevenSpielberg .
```

```
  ?movie mov:genre ?genre .
```

```
  ?movie mov:releaseYear ?releaseYear .
```

Predicates used to retrieve information from the graph

```
  FILTER (?releaseYear > 2000) .
```

Filtering clause that applies a condition to retrieve specific results

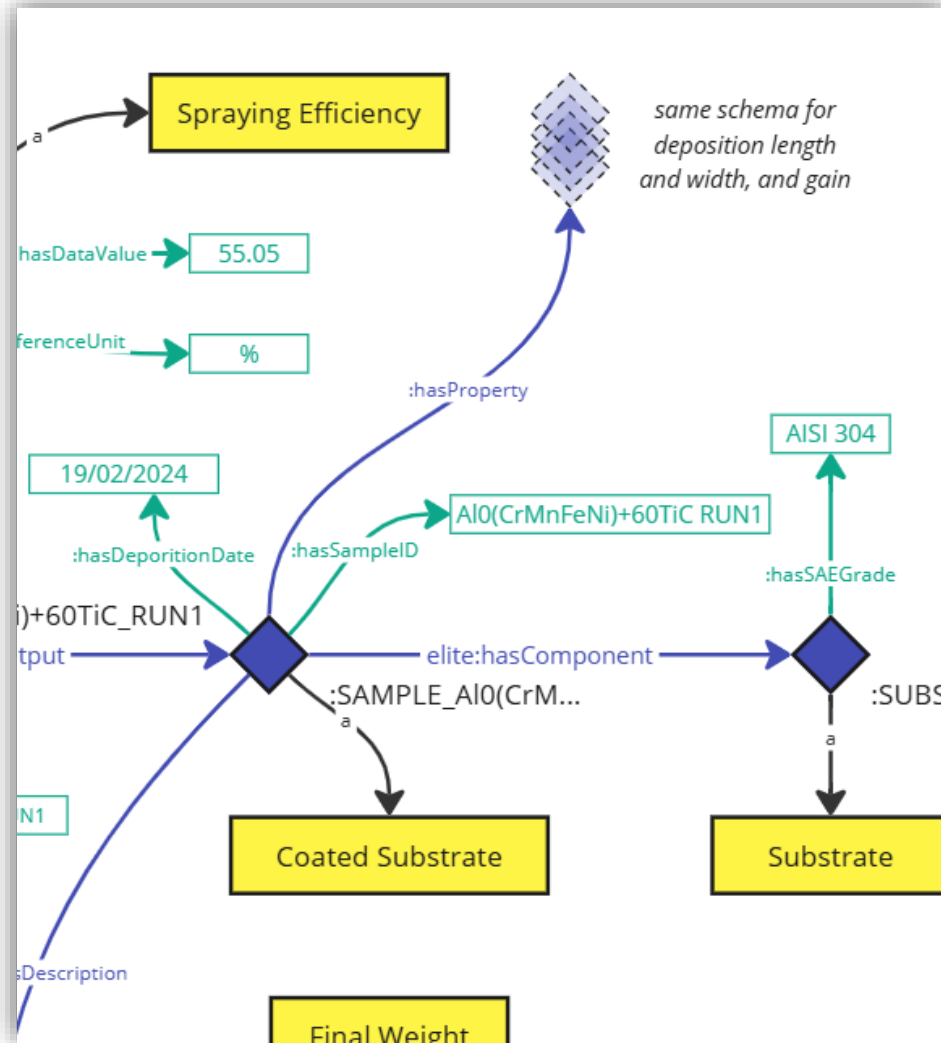
```
}
```

# 4. Analysing

What tools did/will your project develop to extract knowledge from your data?



Conceptual schemes are paramount to elucidate the **CoBRAIN ontology data model** and **concept relations**, in order to enable non-expert users to generate the **correct SPARQL query** for their needs.



## SPARQL Query & Update

Editor only Editor and results Results only

Unnamed x Unnamed x Unnamed 2 x +

```
1 PREFIX owl: <http://www.w3.org/2002/07/owl#>
2 PREFIX : <https://www.cobrain-project.eu/ontology/cobrain#>
3 PREFIX elite: <https://w3id.org/emmo/emmo-lite#>
4 PREFIX xsd: <http://www.w3.org/2001/XMLSchema#>
5
6 select distinct ?pt where {
7   ?s a :CoatedSubstrate .
8   ?s elite:hasProperty ?p .
9   ?p a ?pt .
10  ?pt rdfs:subClassOf elite:Property .
11 } limit 100
```

Press Alt+Enter to autocomplete keyboard shortcuts

Download as

Filter query results Compact view Hide row numbers

Showing results from 0 to 8 of 8. Query took 0.1s, minutes ago.

pt
1 elite:Property
2 cobrain:ThermalSprayingProcessProperty
3 cobrain:Weight
4 cobrain:PlateWeightGain
5 cobrain:DepositionLength
6 cobrain:Length
7 cobrain:DepositionWidth
8 cobrain:Width

# 4. Analysing

What tools did/will your project develop to extract knowledge from your data?



- SPARQL Query Example

GraphDB

Import

Explore

SPARQL

Monitor

Setup

Lab

Help

## SPARQL Query & Update

Unnamed 1 × Unnamed × Unnamed 2 × ⊕

```
1 PREFIX elite: <https://w3id.org/emmo/emmo-lite#>
2 PREFIX cobrain: <https://www.cobrain-project.eu/thermalspraying#>
3 select ?spray_eff_val ?av_peak_t_val where {
4     #want to find the values of spray efficiency
5     ?spray_eff a cobrain:SprayingEfficiency .
6     ?spray_eff elite:hasDataValue ?spray_eff_val .
7     #for a HVOF spraying process
8     ?spray_eff elite:isPropertyOf ?spray_proc .
9     ?spray_proc a cobrain:HVOF .
10    #and compare with the values of average peak temperature
11    ?av_peak_t a cobrain:SubstrateAveragedPeakTemperature .
12    ?av_peak_t elite:isPropertyOf ?coated_sub .
13    ?coated_sub a cobrain:CoatedSubstrate .
14    ?coated_sub elite:isOutputOf ?spray_proc .
15    ?av_peak_t elite:hasDataValue ?av_peak_t_val .
16 } limit 100
```

Run

keyboard shortcuts

CoBRAIn en

Editor only Editor and results Results only

Table Raw response Pivot Table Google Chart

Download as

Filter query results Compact view ☐ Hide row numbers ☐

Showing results from 0 to 2 of 2. Query took 0.1s, moments ago.

	spray_eff_val	av_peak_t_val
1	"60.9686609686609"^^xsd:decimal	"406.3234116948068"^^xsd:float
2	"59.4017094017094"^^xsd:decimal	"387.4334548484541"^^xsd:float

## 4. Analysing

What tools did/will your project develop to extract knowledge from your data?



**CoBRAIN Knowledge Base** will be used mainly to:

- Create a **federated interoperable database** for the CoBRAIN partners that can be used also after the project ends
- Provide **FAIR solution** for the dissemination and exploitation of project data
- Support the creation of a **SDSS** (Sustainable Decision Support System)

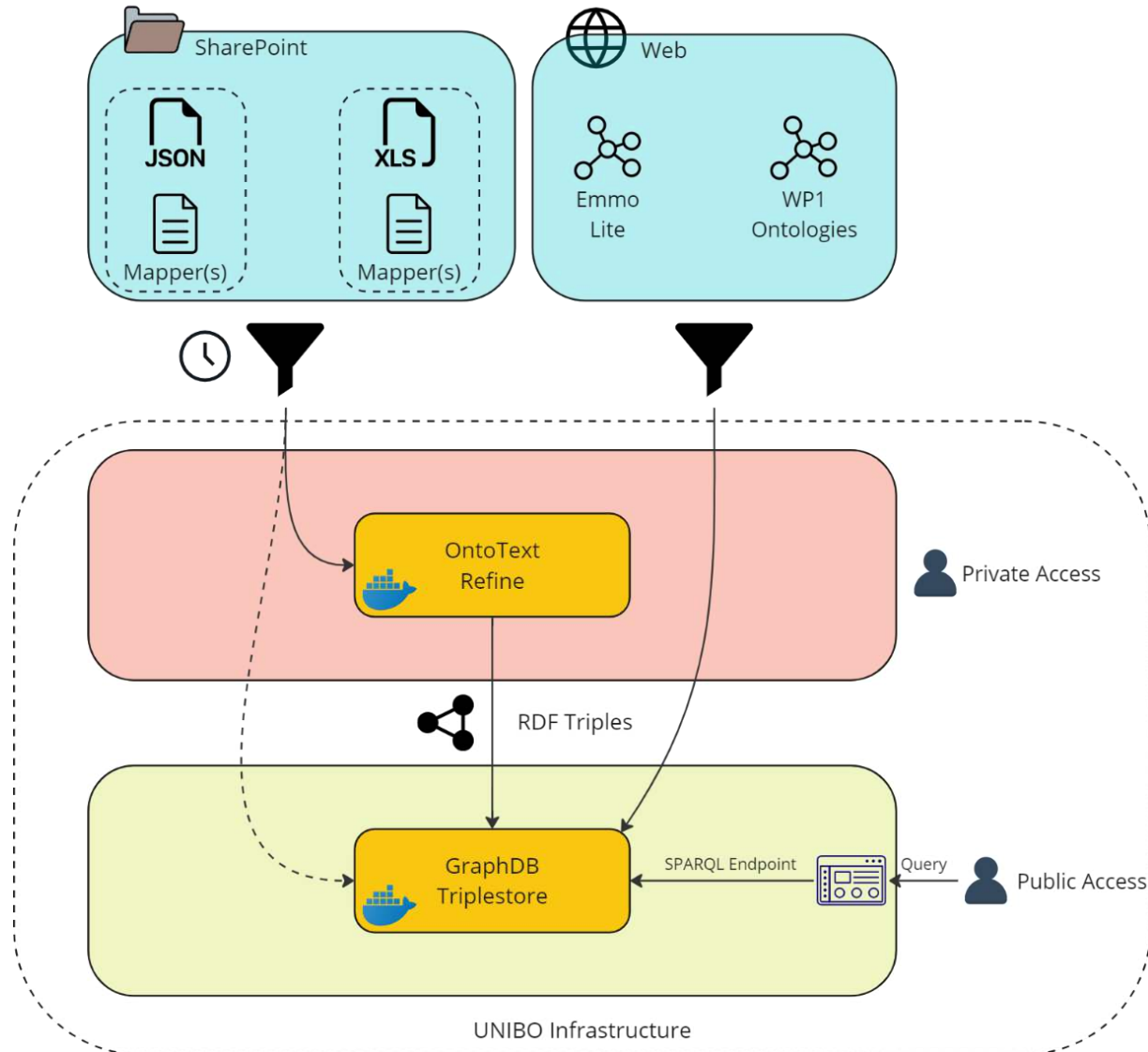
The **CoBRAIN ontology for Thermal Spraying** can be used by other research groups to make their data interoperable with CoBRAIN.



# 5. Preserving

o How do you document your “new” data?  
o Are you using versioning?

o In what sort of repository does the preservation happen?



## Ingestion Point

- Periodic import of experimental data and mappings from the project sharepoint
- Import of EMMO and project ontologies from websites

## OntoTextRefine

- Conversion of raw data into formatted RDF triples
- Automatic saving on triplestore

## GraphDB

- Storing of concepts and individuals with data
- Dashboard for query submission

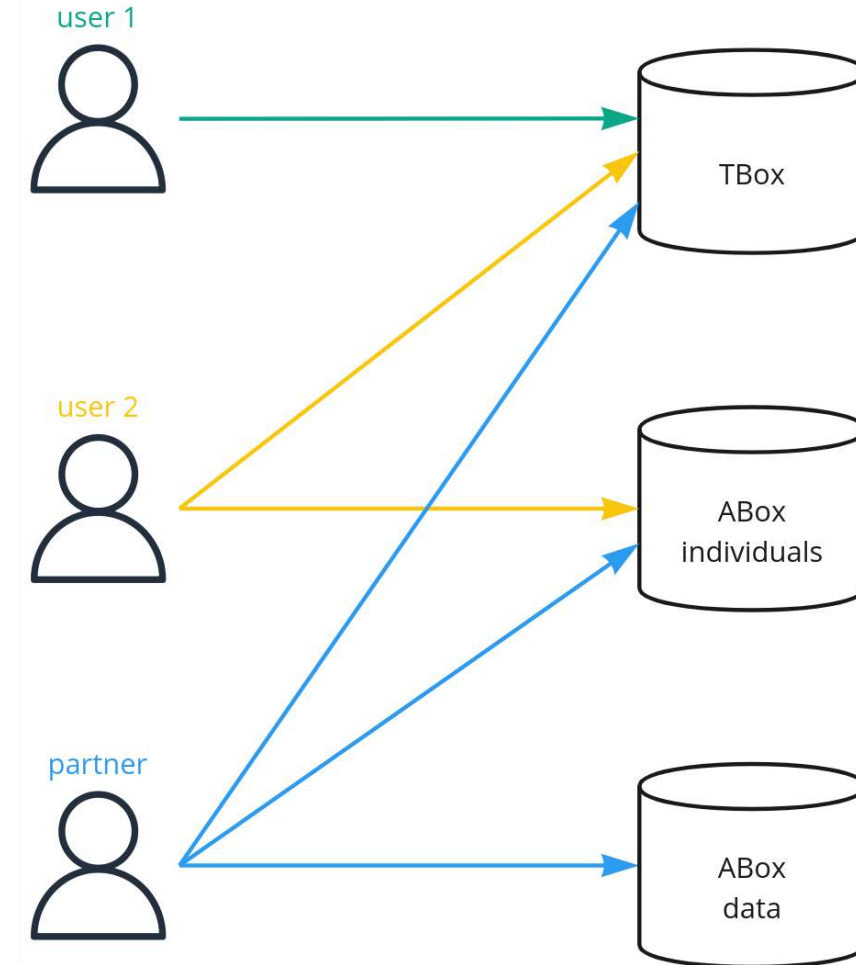
## 6. Sharing

o Are your data sharable with 3rd parties?

o Do you publish your code/Apps/workflows?



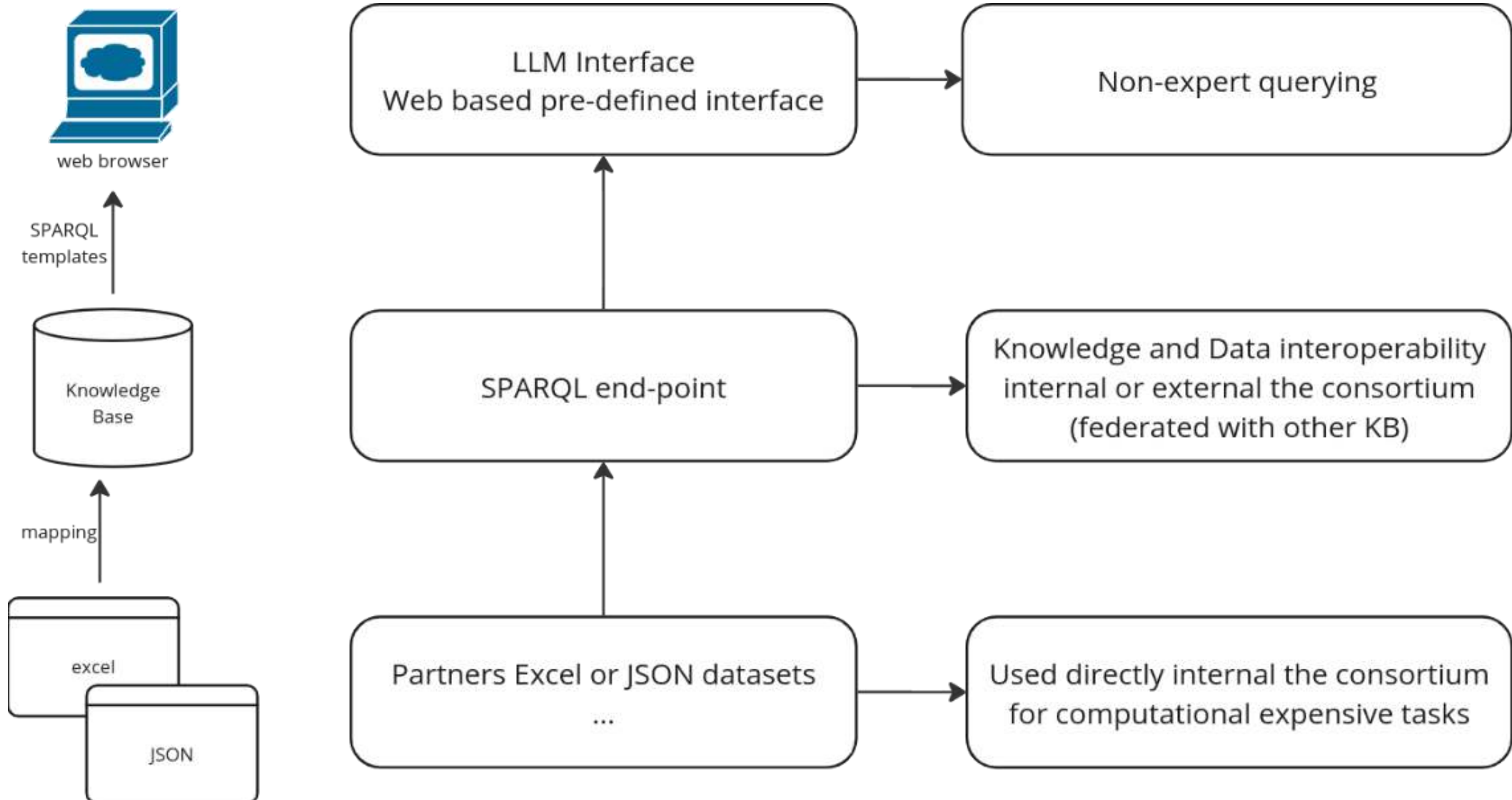
- We identify three distinct types of users, categorized by their access levels:
- **TBox-only users:** These users have access exclusively to the TBox, so the connection between entities.
- **TBox and ABox users:** These users can access the TBox and individuals within the ABox.
- **Partners with full access:** These users have access to the TBox, ABox individuals, and the real data.



## 6. Sharing

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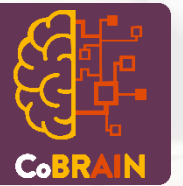


We now have:

- Developed a **fully operable methodology** for the KB, based on the free version of a well-known commercial triplestore (GraphDB) and tools (OntoRefine)
- **Easy to deploy and share** in other frameworks (the overall KB can be shared as a single file, ontology included)
- The TBox is based on **EMMO-LITE** and **CoBRAIN ontology**, usable with OWL 2 RL/QL/EL profiles
- Established a **low-mid level framework** for **FAIR data** in the field of thermal spraying of materials
- Proposed **user-friendly methodologies** for data collection in **experimental environment**
- Provide a **scalable and federated** environment for knowledge management that can be expanded in the future with external DB (e.g. Mongo DB)
- Set of **semantically connected datasets** for interoperable SPARQL queries
- **Knowledge Base** deployed in a test server.



# Our Team - Partners



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**CoBRAIN**

Thank you for your attention!

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Entity: University of Bologna



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the European Union