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Integrated Computational-Experimental Material Engineering of Thermal Spray Coatings

Deliverable D1.4

CoBRAIN Knowledge Base Repository - RDS Triplestore

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[1] PU = PUBLIC fully open ((warning) automatically posted online on the Project Results platforms)

SEN = Sensitive — limited under the conditions of the Grant Agreement

EUCl = EU classified under Decision 2015/444

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Project Profile

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1.0	23/12/2024	UNIBO, UMR	Final Review

Publishable Summary[2]

This deliverable provides a brief description of the CoBRAIN Knowledge Base, deployed by UNIBO to provide a common framework for the data generated during the project activities. The knowledge graph developed in T1.1 has been deployed using GraphDB Desktop Free Edition, a commercial RDF triplestore solution available with a freeware license solution, that provides state of the art capabilities.

The knowledge base hosts:

a) the EMMO-LITE ontology, a lightweight version of the EMMO (Elementary Multi-perspective Material Ontology)[3],

b) the CoBRAIN ontology for thermal spraying, built on the top of the EMMO-LITE

c) a first batch of data from UNIMORE, MBN and ACCESS described in the Data Management Plan covering HVOF/HVAF processes and the characterization and modelling domains.

The Knowledge Base provides a public SPARQL endpoint making the CoBRAIN project data results accessible to the European community under FAIR principles.

[2] This summary will be used for public dissemination of CoBRAIN's activities.

[3] https://github.com/emmo-repo/EMMO

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Abbreviations

Abbreviation	Definition
ACS	Access e. V.
ANX	Aeonx AI
BAL	Balance Technology Consulting GMBH
CA	Consortium Agreement
CHADA	Characterisation Data
DB	Database
DMP	Data Management Plan
EMCC	The European Materials Characterisation Council
EMMC	The European Materials Modelling Council
EMMO	Elementary Multiperspective Material Ontology
EXE	Exelisis IKE
GUI	Graphical User Interface
HHM	High Entropy Hardmetals
HVOF	High Velocity Oxygen Fuel
ISQ	International System of Quantities ISO 80000
KB	Knowledge Base
KME	Knowledge Management Environment
LLM	Large Language Model
MODA	Materials Modelling Data
MBN	MBN NANOMATERIALIA SPA
OTE	Opern Translation Environment
TRL	Technology Readiness Level
UB	Universitat De Barcelona
UMR	Universita Degli Studi Di Modena E Reggio Emilia
UNIBO	Alma Mater Studiorum - Universita Di Bologna
UR3	Universita Degli Studi Roma Tre

1 Introduction

CoBRAIN is a collaborative initiative in the form of a Horizon Europe project that aims to develop novel hard metals for thermal spray coatings based on compositionally complex systems of High Entropy Alloy and Carbides as a binder and hard phase, respectively. A Sustainable Decision Support System will be also developed in the context of the project, to identify specific elements and process solutions optimisations for the CoBRAIN solution to be applied in different scenarios. A unique synergy of the resulting experimental and modelled datasets and data on material lifecycle sustainability will be used in Deep Learning (DL) algorithms to provide support in the decision-making processes for the development of industrial components for different end uses.

The use of **Semantic Web** standards is crucial in establishing a framework of interconnected heterogeneous data sources, facilitating interoperability at both the data and system levels. These standards introduce the idea of **linked data**, shifting from hierarchical structures to network-based organization of data and knowledge. This becomes especially important in scenarios where data is dispersed among different content providers or stakeholders, as is the case for the CoBRAIN datasets, requiring standardized data exchange for effective management of distributed knowledge.

Paramount for the Semantic Web and the concept of linked data is the role of **ontologies**, that have by now established themselves in various hierarchical levels: top-level, middle-level, and domain level. Incorporating top-level ontologies is critical for creating a framework that integrates the other levels. This is especially relevant in dynamically evolving domains like materials science, where new techniques continually emerge. Utilizing top-level ontologies can facilitate a **federation of interoperable databases**, reducing data fragmentation and preventing the formation of data silos.

This approach offers **multiple benefits**: it bridges the disciplinary gap between different domains and helps achieve Industry 5.0 standards, by narrowing the gap between human input and digital tools. It also enhances cross-disciplinary understanding and improves compatibility of domain-specific systems. Importantly, it enhances interoperability between standards, vocabularies, data, and software tools, while allowing more effective data documentation.

Despite these advantages, ontology developers often hesitate to use top-level ontologies, due to the overhead involved. This is further magnified by the fact that terms and approaches in top-level ontologies are not well-understood outside specialized fields, making domain-level ontologies more accessible. Another challenge is the competence bottleneck in formal knowledge representation, as few individuals possess the multidisciplinary skills required for ontology development.

This report describes the result of T1.4 activities that concretize the WP1 efforts of the first two years in the creation of a **Knowledge Base (KB)** based on **GraphDB Desktop Free Edition** triplestore, hosting the CoBRAIN ontological framework based on the EMMO-LITE ontology and a first round of datasets covering HVOF/HVAF processes, characterisation of materials and modelling of microstructures.

It is important to acknowledge that this deliverable presents the efforts undertaken mainly by UNIBO, UMR and MBN, with the valuable support of the overall CoBRAIN consortium.

2 The Knowledge Management Environment

2.1 Introduction

2.1.1 Overall KME Architecture

The overall approach to knowledge management in CoBRAIN can be summarised in Figure 1. It consists of a **KB system** designed to collect user cases and metadata, and to link together datasets that are locally stored by the CoBRAIN partners in their specific storage solution of choice.

This architecture has the benefit of maintaining almost unaltered the existing data collection and storage methodologies that domain experts are using in their technologically relevant environment, since the KB is built on top of them, exploiting the virtualisation techniques that are available in commercial graph databases solutions.

The architecture is fully described in detail in CoBRAIN D1.1.

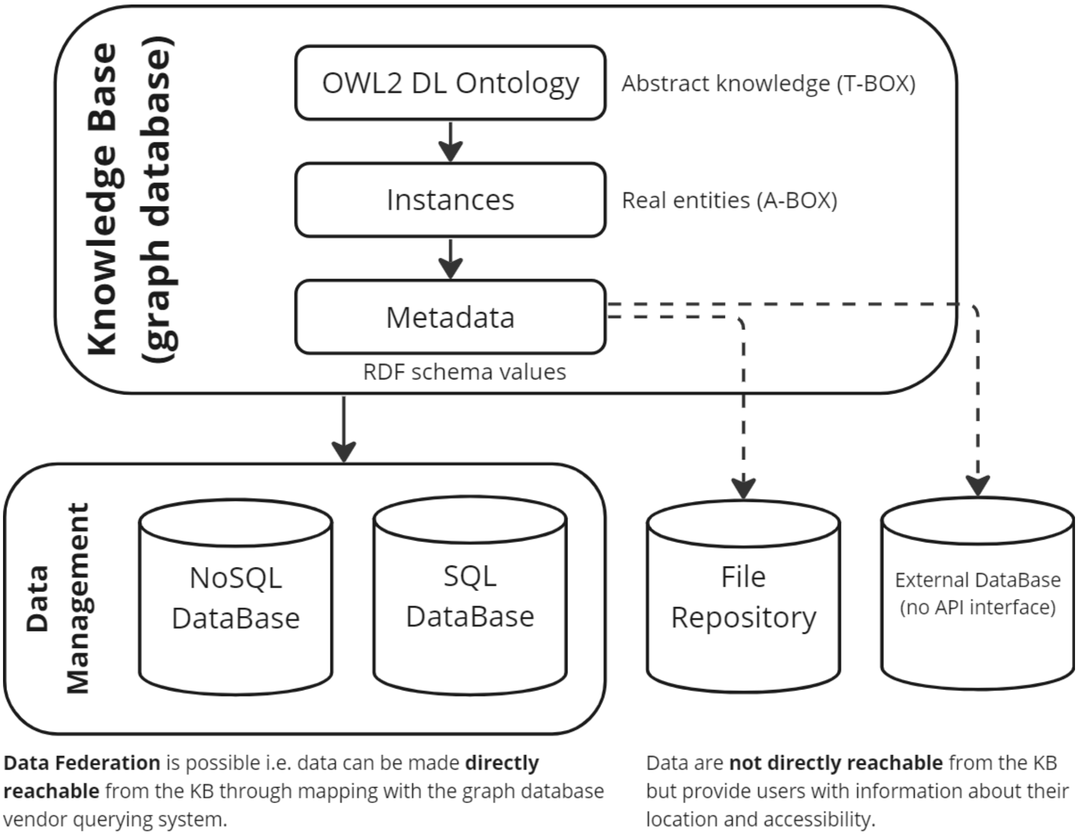
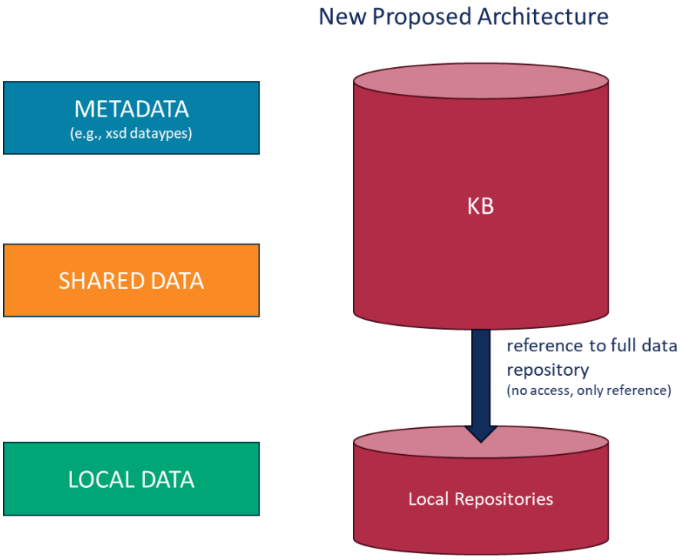


Figure 1 - The overall CoBRAIN KME architecture.

The original architecture **has been simplified during the development phase**, to reduce the data management efforts of the partners. This has been achieved by providing direct mappings between the datasets generated by each partner in different serializations (e.g., JSON, Excel) and the CoBRAIN ontology.

The mappings enabled a direct conversion of the data in RDF triples that can be ingested by the KB, without the need of the virtualisation layer, and simplifying *de facto* the overall data management efforts of the partners. The new architecture is depicted in Figure 2, in which the nanoindentation data are stored directly in the KB. The original data, that have been processed to generate the shared data, are stored locally and only referenced by the KB.

This benefit comes with the cost of an increased effort of UNIBO personnel in terms of maintenance and update of the collection of partners' datasets, together with a periodic update of the Knowledge Base content that will continue during the overall project duration under UNIBO supervision.



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	**mN,** the value of the critical load, identified from Indentation curve: (Load applied [N] vs penetration depth).
K_{IC}	**MPa√m,** 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	**.mss**, located in UNIROMA3's servers, contains all the information related to the measurement and the complete results.
Indentation Data	**.xls**, located in UNIROMA3's servers, contains data, exported from .mss, needed for fracture toughness calculation (i.e. applied load [mN] vs penetration depth [nm]).

Figure 2 - KME and an actual CoBRAIN dataset.

2.1.2 Data Flow and User Interfacing

The KME, whose KB is the most important technological asset, interacts with users at three different levels, as shown in Figure 3. The shared data are available to project partners in local heterogeneous formats (e.g., JSON, Excel), using fixed templates for each dataset, as described in the DMP. These datasets are stored in a shared environment and directly accessible by partners for all user case scenarios where the context for data interpretation is clear and well identified, and KB benefits are not relevant. The standard templates for each format have been provided by UNIBO.

After the dataset ingestion thanks to dataset mapping to the EMMO ontology, the information carried by them is available in the KB through a SPARQL endpoint, remotely accessible on a public server. This method for data retrieval is relevant when users want to retrieve data in an interoperable scenario (e.g., collect characterisation data provided by different partners for the same deposition sample). Moreover, it can be federated with other KBs based on EMMO for a seamless integration with other domains' data.

Finally, it is possible to link a LLM to the KB for the retrieval of data by non-expert users via natural language questions that will be used to rapidly generate SPARQL queries. This feature is not foreseen by the CoBRAIN Grant Agreement but can be implemented as demonstration of semantic technologies benefits, since a LLM can benefit from the semantic enhancement of data to understand what they are about and provide the dataset that better matches the natural language query with the semantic annotations.

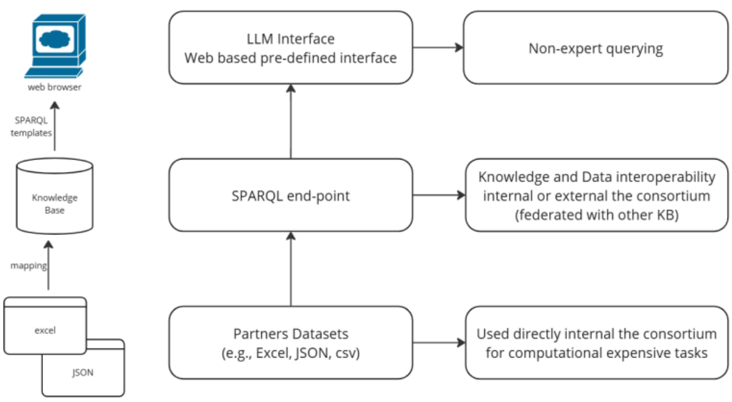


Figure 3 Levels of users' interaction with the KME

2.2 Architecture

This section outlines the infrastructure developed for the CoBRAIN project to enable the processing, storage, and utilisation of experimental data within a knowledge base designed to be queried by the end users. The architecture leverages two advanced tools, OntoText Refine and GraphDB, to automate the transformation of existing data into RDF triples compatible with triplestore technologies, store them, and ensure their accessibility to end users.

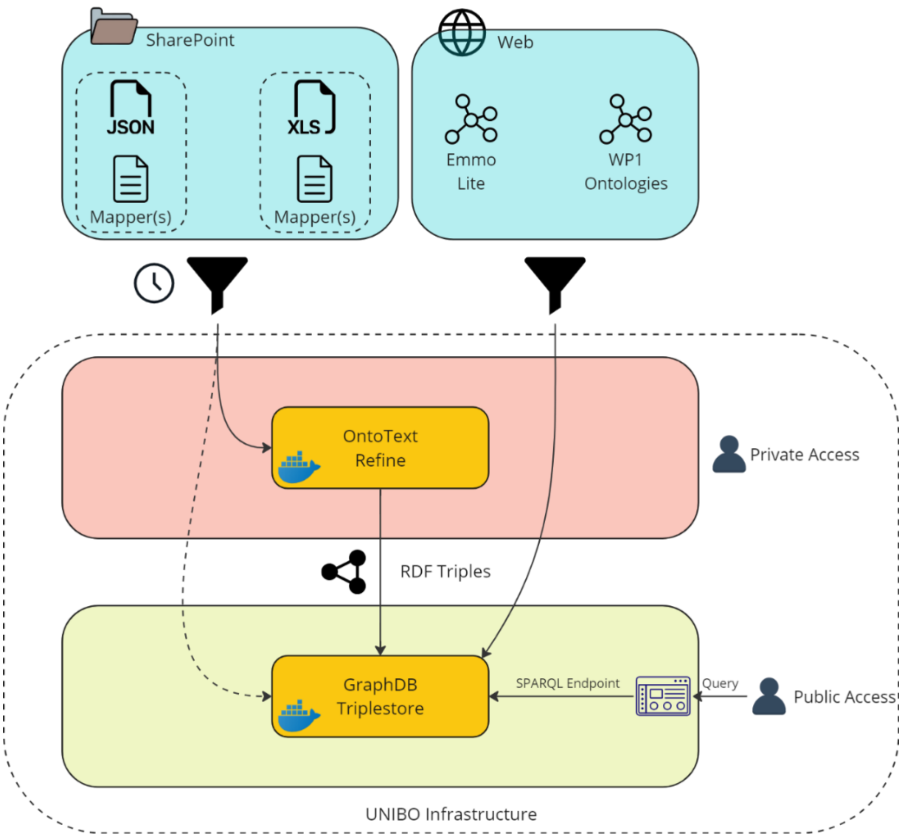


Figure 4 Architectural overview of the infrastructure for the CoBRAIN project.

2.2.1 Architecture Overview

Figure 4 shows the high-level overview of the infrastructure developed for the CoBRAIN project. The structure relies on three main layers: the Ingestion layer, OntoText Refine, and GraphDB.

The Ingestion layer consists of private and public repositories containing information that needs to be inserted into the final knowledge base. This concerns loading the public EMMO and COBRAIN ontologies, and the experimental data that are saved by the partners in the project SharePoint as they are produced. At this level the architecture fetches periodically the new data from the SharePoint and proceeds with the automatic ingestion into the platform.

The OntoText Refine part uses the homonymous tool along with the ingestion scripts to automatically convert the experimental data into RDF triples. This is achieved using mapper files, each specific to a single dataset, which are retrieved from the project SharePoint. It is noteworthy to highlight that these processes are completely hidden from the final user, which can directly interact with the final output of the operations.

Finally, GraphDB serves as a full-fledged triplestore that forms the knowledge base of the project collecting all data coming from the above layers, providing users with an access point that enables the linking of information through SPARQL queries. Furthermore, GraphDB also provides the possibility to manage users by setting permissions and visibility policies for each of them. This is a mandatory feature, since this layer is exposed to the final users via a web interface.

The solution adopts a modular deployment approach using two Docker containers, enabling changes to be implemented with minimal configuration while ensuring platform independence. This structure makes the code highly portable and facilitates the deployment on different machines. More details will be provided into the subsequent sections.

2.2.2 Ingestion Points

The ingestion points represent the data sources from which the infrastructure collect and process information, using the ingestion scripts, to store it in the GraphDB triplestore. In the proposed solution, there are two main ingestion points:

- Public ontologies, accessible via public URLs
- Private data present in the project common share point

The former comprises the EMMO-lite ontology, a branch of the EMMO ontology, and the CoBRAIN ontology specifically developed for the project. The ingestion of this data is done once at the startup of the GraphDB triplestore instance and, currently, any update needs to be pulled manually via the web interface.

On the other hand, the private data present in the project common SharePoint consists of all the experimental datasets produced by the project partners. Each data set is organized by typology and is assumed to have a dedicated folder containing both the raw data and the mapper file for the ontological conversion (see Section 2.2.3). The job takes place in the OntoText Refine Docker container using a cronjob which schedules the execution of the script that periodically checks if new data has been added and, eventually, proceeds with the automatic conversion using the tool.

2.2.3 OntoText Refine

OntoText Refine is a full-fledged technology created to automate the conversion of heterogeneous unstructured or semi-structured data formats, including CSV, XML, JSON and XLSX, into a knowledge graph.

To achieve this, Refine can filter, edit and clean errors or inconsistencies in the input file, and map each of its elements to an ontological described concept. The association is done via a configuration file, called mapper, that contains all the relation between a tabular raw data and its relative RDF triples in terms of subject, object, and predicate. At the end of the process, the mapper will enable the creation of a set of RDF triples to be saved into the GraphDB triplestore automatically.

The mapper needs to be created manually once, then it is possible to use the same schema for each dataset which follows the same structure. Although it comes with a user-friendly web interface, the conversion process can be completely automatized via the Refine CLI, which provides a set of functionalities for processing and converting raw data directly.

Currently, two experimental datasets, the HVOF and Pyrometry from UNIMORE, have been successfully mapped and integrated into the platform for automatic ingestion and storage.

2.2.4 GraphDB

GraphDB is a state-of-the-art triplestore technology that stores ontological information in the form of triples. Among its main features, GraphDB can organize the knowledge based into independent workspaces called repositories. Within each repository, users can upload their triples, eventually subdividing them in named graphs, and interrogate the stored knowledge information through SPARQL queries.

Furthermore, it also comes with a set of management features such as user access control. It supports the creation of users with different permission policies to control logins and allow a differentiated access to the different graphs of the knowledge base. This feature is very valuable to protect sensible or private information such as the triples coming from the experimental dataset, while still allowing the access to the public data like EMMO and CoBRAIN public ontologies.

In the CoBRAIN project, GraphDB is used as main triplestore technology to save all the information coming from the ingestion points. From a structural perspective, we decided to separate each different dataset into a different named graph inside a single global repository named “cobrain”. This separation enables a differentiated access when it comes to separate public data from private ones. Figure 5 illustrates the named graphs present currently in the infrastructure including those for the EMMO, cobrain and HVOF dataset ontologies.

Furthermore, the access to the information is exposed via a web dashboard which exposes a user-friendly text editor to allow end users to create and submit SPARQL queries (Figure 6). On the other side, the access to the raw SPARQL endpoint enables expert users to interact with the knowledge base programmatically via scripts, so that high-level functionalities can be easily implemented.

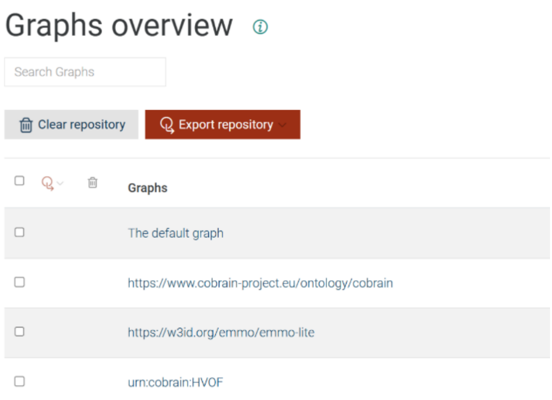


Figure 5 Named Graphs structure for the CoBRAIN repository.

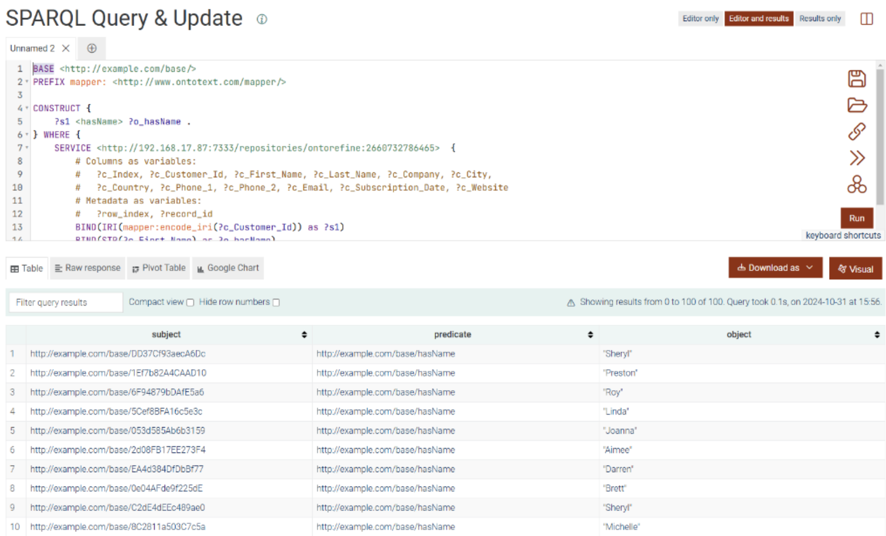


Figure 6 SPARQL Editor in the GraphDB dashboard.

2.2.5 Deployment

The deployment of the infrastructure leverages two main Docker containers, built from the official OntoText Refine and GraphDB images. These images have been modified to include functionality tailored for the project’s needs, such as the graph initialization and the ingestion scripts execution.

Specifically, the Refine image has been modified to enable the *cron* daemon and, in doing so, enabling the periodic execution of the ingestion scripts. This setup ensures that the script for each dataset category, as detailed in Section 2.2.1, is automatically executed on a regular schedule. Similarly, the GraphDB image has been modified to automatically create the CoBRAIN repository inside the triplestore and collect all the ontologies related to EMMO-LITE and CoBRAIN to save them in the proper named graph.

Future developments will include the addition of new ingestion scripts as new experimental datasets will be provided, and the automatic management of user definition and knowledge base partition in the GraphDB repository.

2.2.6 Usage

To interact with GraphDB, a registered user starts by logging in to the platform using their username and password.

After logging in, the user may have different available tools based on their permissions, the most important tool is the SPARQL query editor, that provides a comfortable UI allowing the user to write and run SPARQL queries after selecting the desired repository.

When the query is executed, the results will appear under the editor. They can be downloaded in different formats, such as JSON and CSV, and the frequently used queries can be saved for future use.

3 Dataset Mapping

3.1 CoBRAIN Ontology

The CoBRAIN ontology has been extensively described in D1.1. The ontology is available in the KB, together with the EMMO-LITE module upon which it depends, as shown in Figure 7

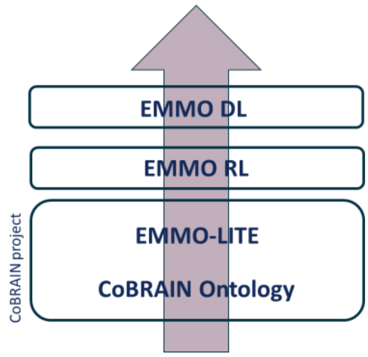


Figure 7 CoBRAIN Ontology Dependencies

The CoBRAIN ontology is publicly available via the CoBRAIN GitHub public repository https://github.com/cobrain-project/ontology and constantly updated to match the applications and user's needs. Each DMP dataset requires an ontology extension to cover its specific concepts that were not initially considered. The ontology update will last up to the end of the project according to users' feedback.

For example, all CoBRAIN coating materials have been added to the ontology by extending the EMMO-LITE Material branch according to the materials specifications. These concepts will be used to specify the type of powders used in each deposition run with different spraying technologies (e.g., HVOF, HVAF, Cold Spraying). The material hierarchy is shown in Figure 8. Each material class carries annotations and axioms on data properties that link material individuals to each specific type according to composition or common nomenclature, as shown in Figure 9.

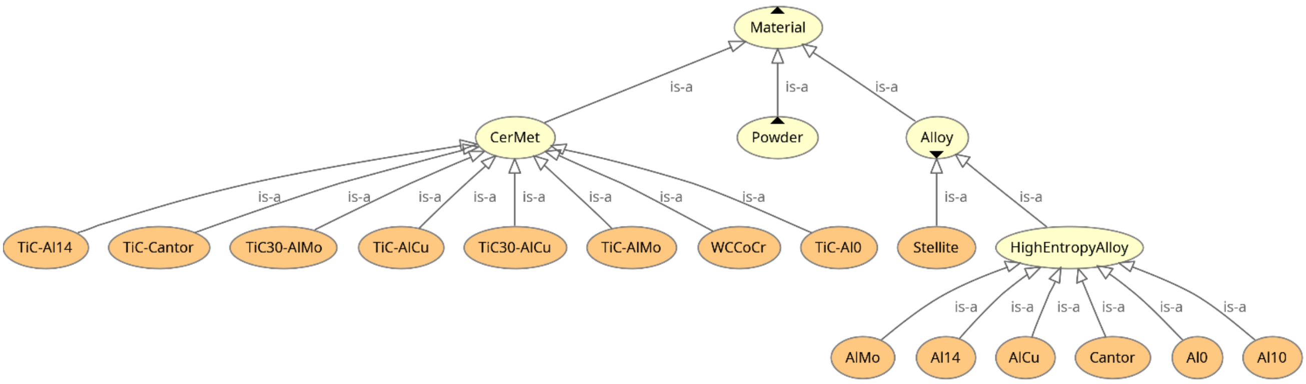


Figure 8 CoBRAIN materials taxonomy.

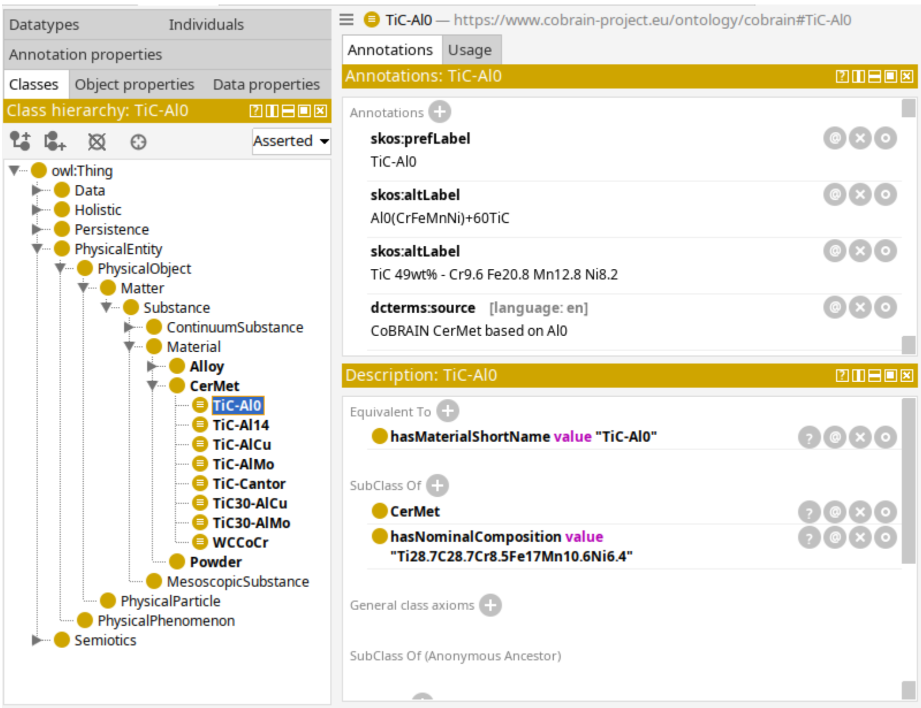


Figure 9 Example of axiomatic description of a CoBRAIN material class.

3.2 Conceptualisation Mappings

Dataset mappings to the EMMO based CoBRAIN ontology are provided to users via conceptual boards, using MIRO collaboration platform, to represent visually the relations between all data made available by each dataset. This boards (once per dataset) can be used by users that have no deep understanding of the CoBRAIN and EMMO ontology to create queries for knowledge retrieval from the KB. Moreover, the boards are a useful design tool for OntoRefine dataset mapping.

Some examples of mappings are provided in the next section, to facilitate the understanding of the approach.

3.2.1 UMR HVOF Thermal Spraying Logbook

This dataset refers to the High Velocity Oxygen Fuel (HVOF) Thermal Spray Logbook from UMR partner, as described at p. 41 of the DMP. The conceptual mapping is shown in Figure 10, and provides relations between all data provided by the Excel dataset shown in Figure 11.

The board shows data properties as green arrows (i.e., data directly connected to an individual), that provides immediate, semantically trivial, information for each entity. For example, the date of a particular deposition, material nomenclature (e.g., AISI 304), the value of a property.

The object properties (i.e., semantically relevant relations) are shown as blue arrows connecting individuals, and provide information about the processes steps, the component of a system, the semiotic relation between a physical quantity (e.g., the spraying efficiency) and the entity for which it stands (e.g., the HVOF process).

Each individual type is shown by connecting the individual with a yellow box showing the class name through a black arrow that stands for the *rdf:type* relation (customarily abbreviated as "*a*"). The yellow classes are defined in the CoBRAIN ontology.

The dark blue diamonds represent concrete individuals that are part of the KB A-Box with their IRIs, while light blue diamonds represent blank nodes i.e., individuals that are not explicitly declared but are identified according to their relations. For example, properties such as feed rate are not declared as concrete individuals but as an entity that has a value and a reference unit.

The mapping, graphically elucidated by the board, is also formally expressed using the OntoRefine GUI as shown in Figure 12, which enables the conversion of the dataset template format (e.g., Excel, JSON) in an RDF serialisation to be loaded into the KB triplestore.

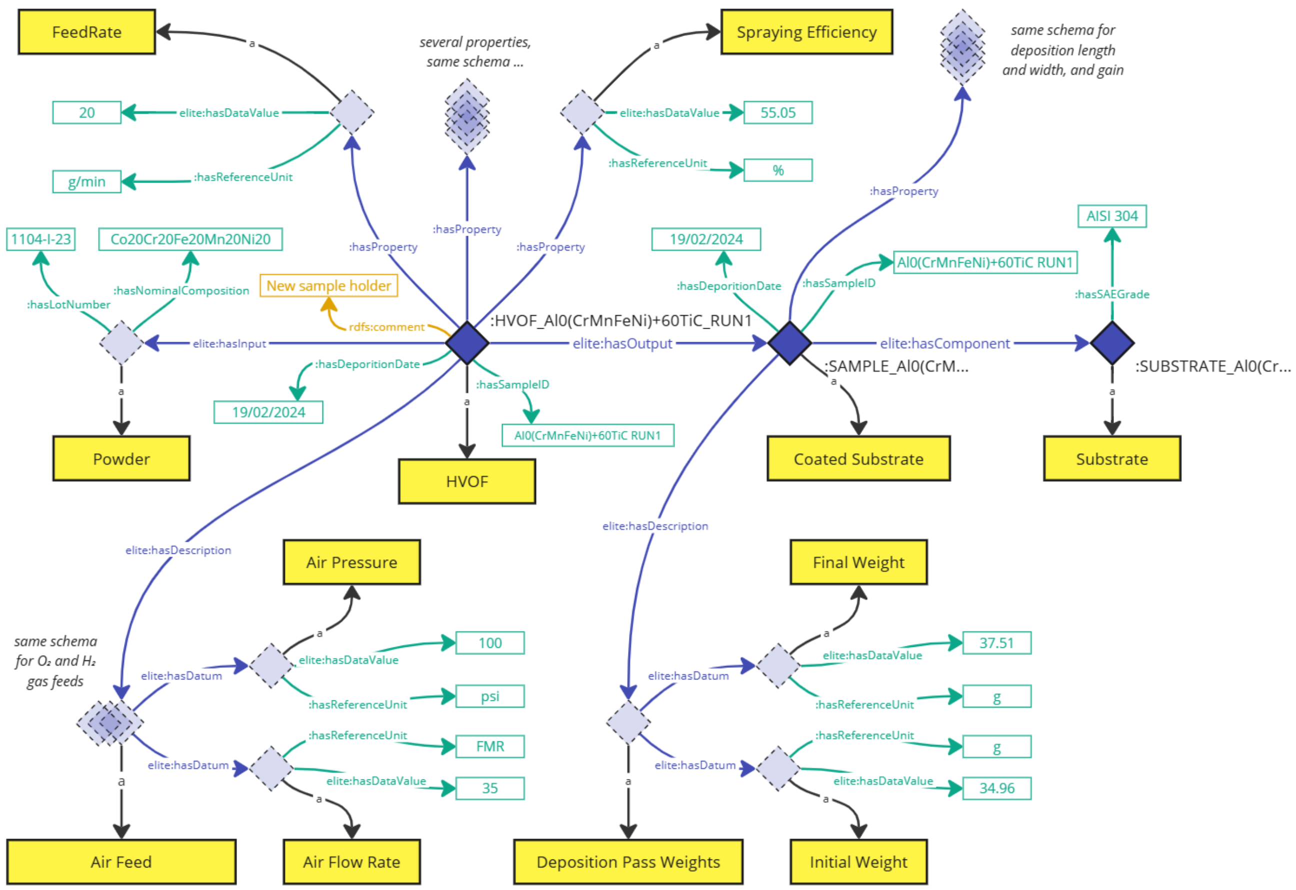


Figure 10 Conceptual Mapping of UMR HVOF Thermal Spraying Logbook

POWDER		SUBSTRATE	COATED SUBSTRATE			HVOF													COATED SUBSTRATE							HVOF		
Nominal Composition	Lot. N.	SAE Grade	Sample ID	deposition area length [mm]	deposition area width [mm]	FR H_2 [FMR]	p H_2 [psi]	FR O_2 [FMR]	p O2 [psi]	FR Air [FMR]	p Air [psi]	Pwdr. Feed [g/min]	Standoff [mm]	Pitch [mm]	Speed [mm/s]	n° cycles	n° passes/cycle	n° preheat 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 [%]	Notes
Co20Cr20Fe20Mn20Ni20	209-C-23	AISI 304	Cantor RUN1	54	25	56	140	30	170	35	100	30	250	5	750	9	3	3	34.96	37.51	35.18	37.27	34.85	37.60	2.46	4.86	50.69	
Co20Cr20Fe20Mn20Ni20	209-C-23	AISI 304	Cantor RUN2	54	25	56	140	30	170	35	100	20	250	5	750	13	3	3	35.18	37.88	35.25	37.62	34.95	37.57	2.56	4.68	54.77	
Co20Cr20Fe20Mn20Ni20	209-C-23	AISI 304	Cantor RUN3	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.25	37.76	35.01	37.57	34.85	37.93	2.54	4.68	54.17	
Co20Cr20Fe20Mn20Ni20	209-C-23	AISI 304	Cantor RUN4	54	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.46	37.43	34.89	37.95	35.22	38.30	3.02	4.68	64.42	
Al14(Cr20Mn25Fe40Ni15)86	343-C-23	AISI 304	Al14(CrMnFeNi) RUN1	54	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34.84	37.21	35.04	37.48	35.00	37.53	2.45	4.68	52.28	
Al14(Cr20Mn25Fe40Ni15)86	343-C-23	AISI 304	Al14(CrMnFeNi) RUN2	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.17	37.57	34.76	37.08	34.58	36.93	2.36	4.68	50.43	
Al14(Cr20Mn25Fe40Ni15)86	343-C-23	AISI 304	Al14(CrMnFeNi) RUN3	54	25	64	140	34	170	35	100	20	250	5	750	13	3	3	35.16	37.70	35.21	37.61	34.77	37.20	2.47	4.68	52.78	
40vol.% (Co20Cr20Fe20Mn20Ni20)+ 60vol.%TiC	396-D-23	AISI 304	Cantor+60TiC RUN1	54	25	56	140	30	170	35	100	20	250	5	750	13	3	3	35.07	37.61	34.75	37.20	34.91	37.36	2.48	4.68	52.99	
40vol.% (Co20Cr20Fe20Mn20Ni20)+ 60vol.%TiC	396-D-23	AISI 304	Cantor+60TiC RUN2	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.30	38.09	35.23	38.13	34.80	37.70	2.85	4.68	60.79	
40vol.% (Co20Cr20Fe20Mn20Ni20)+ 60vol.%TiC	396-D-23	AISI 304	Cantor+60TiC RUN3	54	25	64	140	34	170	35	100	20	250	5	750	13	3	3	35.19	37.87	35.23	38.01	35.06	37.82	2.73	4.68	58.33	
40vol.% (Co20Cr20Fe20Mn20Ni20)+ 60vol.%TiC	396-D-23	AISI 304	Cantor+60TiC RUN4	54	25	62	140	32	170	35	100	20	250	10	750	39	2	2								4.68		*"Low-stress" torch kinematics with doubled pitch distance and alternate back-and-forth cycles so that two complete passes result in 50% pass overlap and are equvalent to a single torch pass with "standard" torch kinematics*
Al0(Cr20Mn25Fe40Ni15)100	568-E-23	AISI 304	Al0(CrMnFeNi) RUN1	54	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34.38	37.23	34.83	37.72	34.82	37.64	2.85	4.68	60.97	
Al0(Cr20Mn25Fe40Ni15)100	568-E-23	AISI 304	Al0(CrMnFeNi) RUN2	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.27	38.02	35.12	37.93	34.72	37.63	2.78	4.68	59.40	
Al0(Cr20Mn25Fe40Ni15)100	568-E-23	AISI 304	Al0(CrMnFeNi) RUN3	54	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.40	37.08	34.55	37.18	35.09	37.61	2.66	4.68	56.73	
Al14(Cr20Mn25Fe40Ni15)86	343-C-23	AISI 304	Al14(CrMnFeNi) RUN4	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.30	37.74	34.78	37.20	34.73	37.28	2.43	4.68	51.92	*The new sample holder has been used in this experiment to compare the sheer influence of the sample holder alone*
Al14(Cr20Mn25Fe40Ni15)86+60vol.%TiC	1084-I-23	AISI 304	Al14(CrMnFeNi)+60TiC RUN1	60	25	56	140	30	170	35	100	20	20	5	750	13	3	3	34.56	37.75	34.38	37.86	34.24	37.41	3.34	5.20	64.13	*New sample holder*
Al14(Cr20Mn25Fe40Ni15)86+60vol.%TiC	1084-I-23	AISI 304	Al14(CrMnFeNi)+60TiC RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	34.33	37.20	34.47	37.37	34.65	37.54	2.89	5.20	55.48	*New sample holder*
Al14(Cr20Mn25Fe40Ni15)86+60vol.%TiC	1084-I-23	AISI 304	Al14(CrMnFeNi)+60TiC RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.52	37.41	34.48	37.42	34.63	37.55	2.92	5.20	56.06	*New sample holder. Irregular spray pause interval*
Al10(Cr20Mn25Fe40Ni15)90	1104-I-23	AISI 304	Al10(CrMnFeNi) RUN1	54	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34.07	36.85	34.36	37.17	34.65	37.41	2.80	4.68	59.72	*New sample holder*
Al10(Cr20Mn25Fe40Ni15)90	1104-I-23	AISI 304	Al10(CrMnFeNi) RUN2	54	25	62	140	32	170	35	100	20	250	5	750	13	3	3	34.65	37.34	34.36	37.05	34.77	37.16	2.69	4.68	57.48	*New sample holder*
Al10(Cr20Mn25Fe40Ni15)90	1104-I-23	AISI 304	Al10(CrMnFeNi) RUN3	54	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.57	37.23	34.46	37.09	34.48	37.17	2.65	4.68	56.52	*New sample holder*
Al14(Cr20Mn25Fe40Ni15)86+60vol.%TiC	1084-I-23	AISI 304	Al14(CrMnFeNi)+60TiC RUN4	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.48	37.44	34.54	37.52	34.83	37.74	2.97	5.20	57.12	*New sample holder*
Al0(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	Al0(CrMnFeNi)+60TiC RUN1	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	34.67	37.76	34.35	37.50	34.26	37.35	3.11	5.20	59.81	*New sample holder*
Al0(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	Al0(CrMnFeNi)+60TiC RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	34.77	37.81	34.89	37.94	34.79	37.86	3.05	5.20	58.72	*New sample holder*
Al0(Cr20Mn25Fe40Ni15)86+60vol%TiC	1364-N-23	AISI 304	Al0(CrMnFeNi)+60TiC RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.80	37.73	34.85	37.76	35.03	37.86	2.89	5.20	55.58	*New sample holder. Slightly irregular feed during the first 2 cycles*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN1	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	35.16	38.27	34.32	37.47	35.25	38.33	3.11	5.20	59.87	*New sample holder. Slightly irregular feed during the first 2 cycles*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN1	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	35.16	38.27	34.32	37.47	35.25	38.33	3.113	5.2	59.9	*New sample holder. Slightly irregular feed during the first 2 cycles*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.07	38.08	34.62	37.47	35.10	38.11	2.96	5.20	56.86	*New sample holder. Slightly irregular feed*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.84	37.74	34.85	37.69	34.13	36.98	2.86	5.20	55.06	*New sample holder. Slightly irregular feed during the first 7 cycles*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN3	60	25	56	140	30	170	35	100	20	250	10	750	39	2	2	34.68	37.77	34.82	37.99	35.10	38.27	3.14	5.20	60.45	*New sample holder.*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.07	38.08	34.62	37.47	35.1	38.11	2.957	5.2	56.9	*New sample holder. Slightly irregular feed*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.84	37.74	34.85	37.69	34.13	36.98	2.863	5.2	55.1	*New sample holder. Slightly irregular feed during the first 7 cycles*
Al9Cr18Cu18Fe18Ni36+60vol%TiC	072-A-24	AISI 304	AlCuCrFeNi+60TiC RUN4	60	25	56	140	30	170	35	100	20	250	10	750	39	2	2	34.68	37.77	34.82	37.99	35.1	38.27	3.143	5.2	60.4	*New sample holder.*
Al3Cr6Fe31Ni34Mo26	368-E-24	AISI 304	AlCrFeMoNi RUN1	60	25	66	140	35	170	33	100	20	250	5	750	13	3	3	35.15	35.48	34.68	36.55	34.59	34.96	0.857	5.2	16.5	*New sample holder. Coatings frequently delaminated.*
Al3Cr6Fe31Ni34Mo26	368-E-24	AISI 304	AlCrFeMoNi RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	34.92	36.45	34.66	36.72	34.99	36.85	1.817	5.2	34.9	*New sample holder. Feed hose leakage (actual feed rate lower than indicated). Surface appearance anyway very poor, as if particles mostly unmelted.*
Al3Cr6Fe31Ni34Mo26	368-E-24	AISI 304	AlCrFeMoNi RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	34.44	36.72	35.21	37.48	34.83	37.15	2.29	5.2	44.0	*New sample holder.*
Al3Cr6Fe31Ni34Mo26+60vol%TiC	383-E-24	AISI 304	AlCrFeMoNi+60TiC RUN1	60	25	56	140	30	170	35	100	20	250	5	750	13	3	3	35	38.1	34.98	38.17	34.95	38.18	3.173	5.2	61.0	*New sample holder. Slightly unstable feed in the first cycle.*
Al3Cr6Fe31Ni34Mo26+60vol%TiC	383-E-24	AISI 304	AlCrFeMoNi+60TiC RUN2	60	25	62	140	32	170	35	100	20	250	5	750	13	3	3	35.29	38.05	35.09	37.92	35.06	37.85	2.793	5.2	53.7	*New sample holder. Slightly unstable feed in the first 7 cycles.*
Al3Cr6Fe31Ni34Mo26+60vol%TiC	383-E-24	AISI 304	AlCrFeMoNi+60TiC RUN3	60	25	64	140	34	170	35	100	20	250	5	750	13	3	3	35.05	38.13	35.06	38.14	35.17	38.21	3.067	5.2	59.0	*New sample holder. Slightly unstable feed.*

Figure 11 Excel Template for UMR HVOF Thermal Spraying Logbook

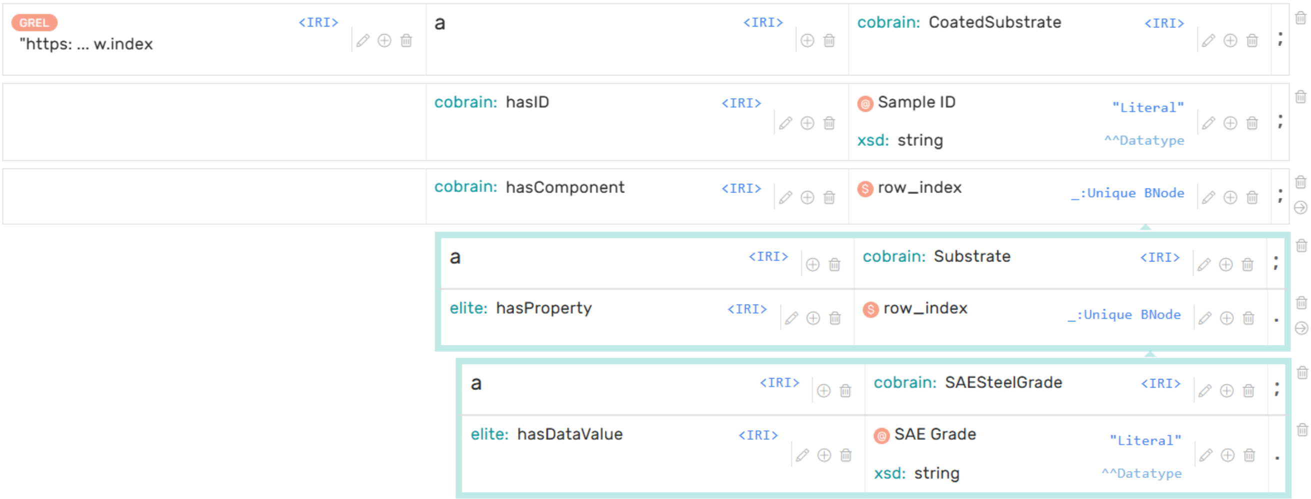


Figure 12 Example of OntoRefine Mapping of UMR HVOF Thermal Spraying Logbook

3.2.2 UMR Optical pyrometer Luchsinger OPTRIS CTlaser

This dataset refers to the Optical pyrometer Luchsinger OPTRIS CTlaser – substrate temperature monitoring during HVOF spraying from UMR as described at p. 42 of the DMP.

This dataset introduces the concept of characterisation and shows how it is expressed via the EMMO framework as a semiotic tetrahedron connecting the measurer, the property, the sample and the measuring process itself, using semiotic-based object property relations. The conceptualisation is graphically elucidated in Figure 13. With respect to the previous case, the board also provides a taxonomical context for the characterisation classes, to let the user understand how they fit the more general EMMO representational framework of characterisation techniques.

The original dataset is stored by UMR partner as JSON file as shown in Figure 14, while the OntoRefine mapping is briefly shown in Figure 15.

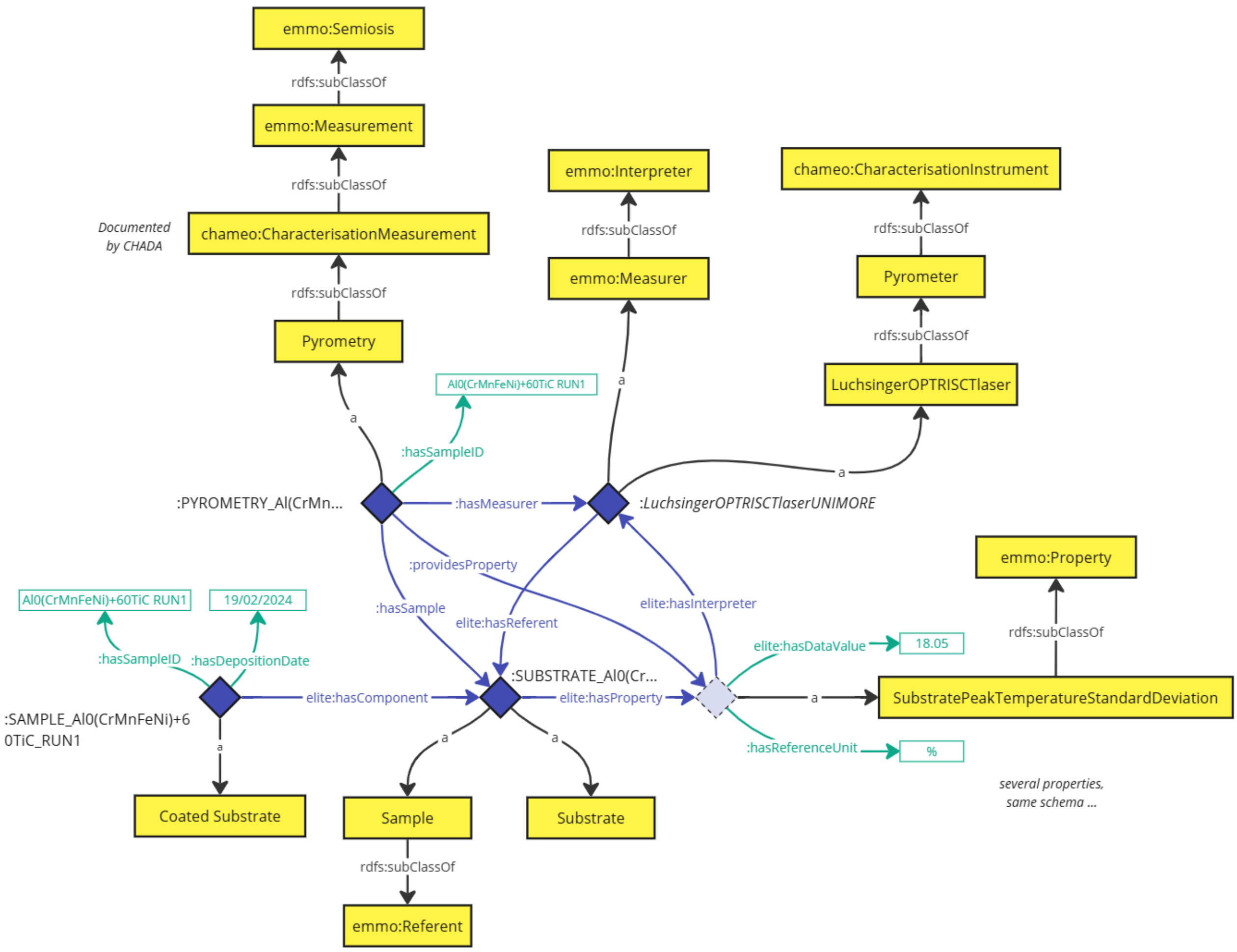


Figure 13 Mapping of UMR Optical pyrometer Luchsinger OPTRIS CTlaser


```json
{
  "Sample_ID": "Al0CrMnFeNi+60TiC Run1",
  "Deposition_date_yyyymmdd": "20240219",
  "temperature_unit": "°C",
  "temperature_peaks": [
    336.54271880497373,
    366.30293803687368,
    374.24048595485141,
    381.061535006703,
    380.0039857820268,
    379.80328491833444,
    380.66470183315317,
    383.10089223240249,
    383.41467060345411,
    381.914551279205,
    380.40849005725835,
    380.684042240002,
    384.06448479994913
  ],
  "average_of_last_5_temperature_maxima": 382.26452186871188,
  "standard_deviation_of_last_5_temperature_maxima": 1.5051560322127098
}
```


Figure 14 JSON Structure for UMR Optical pyrometer Luchsinger OPTRIS CTlaser

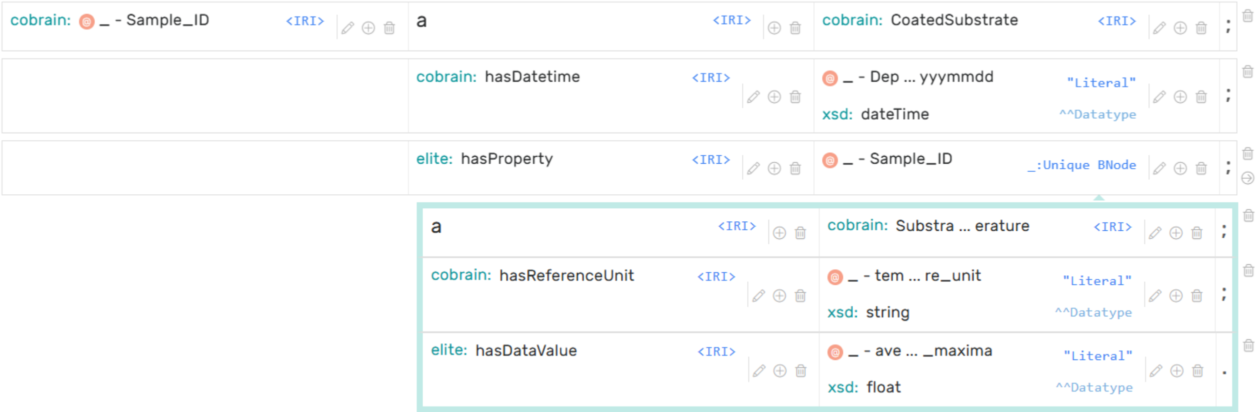


Figure 15 Fragment of the OntoRefine Mapping for the UMR Optical pyrometer Luchsinger OPTRIS CTlaser

3.2.3 MBN HVAF and Blasting Thermal Spraying Logbook

The conceptual mapping of the High Velocity Air Fuel (HVAF) Thermal Spray Logbook from MBN, described at p. 45 of the DMP, is shown in Figure 16.

With respect to previous boards, it shows the sequence of grit blasting and HVAF processes, that are connected using the *elite:isBefore* relation, making this dataset more complex than the previous ones. The board provides a mapping for two Excel datasets: blasting and HVAF. The latter is depicted in Figure 17.

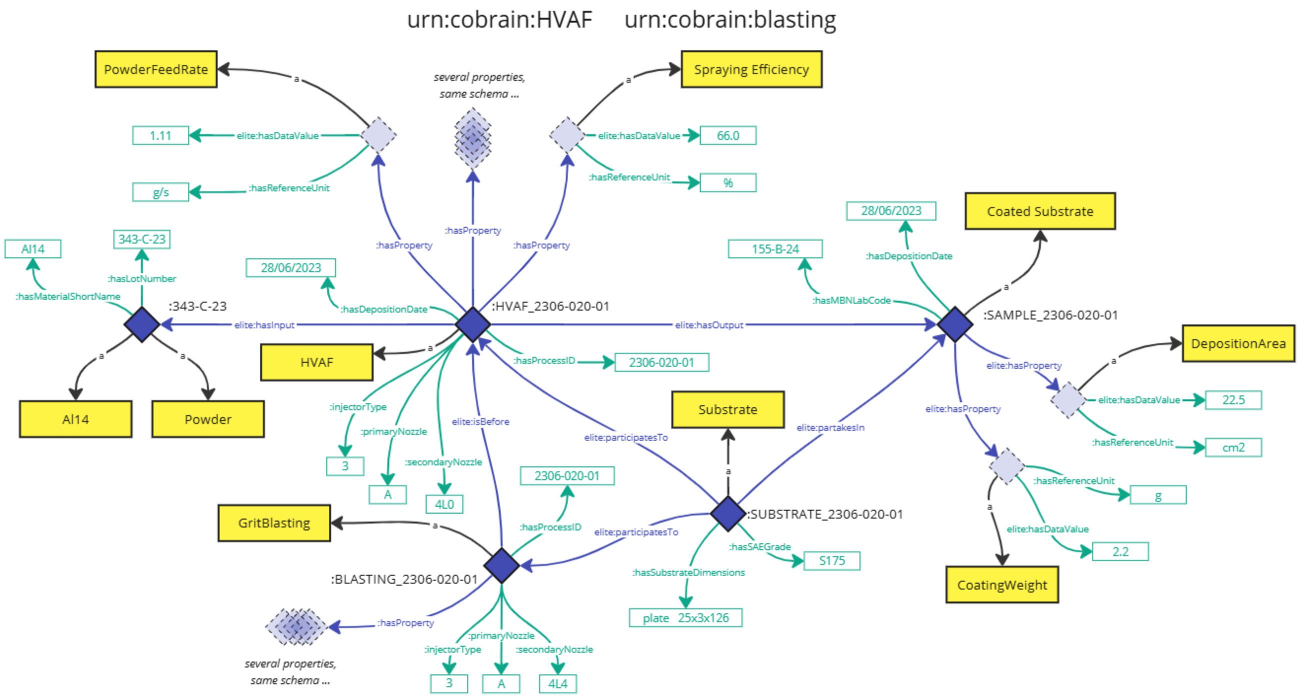


Figure 16 Mapping of MBN HVAF and Blasting Thermal Spraying Logbook

SUBSTRATE				POWDER		HVAF																				COATED SUBSTRATE		HVAF
Substrate Dimensions	Substrate Material	MBN Lab Code	N. of Specimen	Material Short Name	Batch reference (aka Lot Number)	Process ID	Date	N. of Deposition Layers	Pitch [mm]	V [m/s]	Stand Off [mm]	Injector Type	Nozzle Primary	Nozzle Secondary	Air [psi]	Carrier (N2) [slpm]	Fuel (GPL) 1st Stage [psi]	Fuel (GPL) 2nd Stage [psi]	Fuel (GPL) Total [slpm]	Fuel (GPL) Total [l/cm2 x layer (liquid state)]	Carrier (N2) [l/cm2 x layer (liquid state)]	Process Time [s/cm2 x layer]	Nominal Electricity Consumption [kWh/cm2 x layer]	Powder Flow [g/s]	Feedstock Use [g/cm2 x layer]	Deposition Area [cm2]	Coating Weight [g]	Deposition Efficiency [%]
plate 25x3x126	S175		1	Al14	343-C-23	2306-020-01	28 June 2023	4	3.00	1.00	300	3	A	4L0	109	80	97	110	240	0.000108	0.000319	0.03	0.001	1.11	0.04	22.5	2.20	66.0%
plate 25x3x126	S175		1	Al14	343-C-23	2306-020-02	28 June 2023	4	3.00	1.00	300	3	A	4L0	109	55	97	110	240	0.000108	0.000220	0.03	0.001	1.00	0.03	22.5	1.70	56.7%
plate 25x3x126	S175		1	Al14	343-C-23	2306-020-03	28 June 2023	4	3.00	1.00	300	3	A	4L0	107	80	104	87	240	0.000108	0.000319	0.03	0.001	1.37	0.05	22.5	2.10	51.0%
plate 25x3x126	S175		1	Al14	343-C-23	2306-020-04	28 June 2023	4	3.00	1.00	300	3	A	4L0	107	55	104	87	240	0.000108	0.000220	0.03	0.001	1.16	0.04	22.5	1.60	46.1%
plate 25x3x126	S175		1	Al14	343-C-23	2306-020-05	28 June 2023	4	3.00	1.00	300	3	A	4L0	108	50	96	70	240	0.000108	0.000200	0.03	0.001	0.48	0.02	22.5	0.70	48.1%
plate 25x3x126	S175		1	CANTOR + 60%TiC	396-D-23	2306-021-01	29 June 2023	4	3.00	1.00	300	3	A	4L0	109	80	95	110	240	0.000108	0.000319	0.03	0.001	1.21	0.04	22.5	2.00	55.3%
plate 25x3x126	S175		1	CANTOR + 60%TiC	396-D-23	2306-021-02	29 June 2023	4	3.00	1.00	300	3	A	4L0	109	55	95	110	240	0.000108	0.000220	0.03	0.001	0.85	0.03	22.5	1.60	62.7%
plate 25x3x126	S175		1	CANTOR + 60%TiC	396-D-23	2306-021-03	29 June 2023	4	3.00	1.00	300	3	A	4L0	107	80	104	87	240	0.000108	0.000319	0.03	0.001	0.83	0.03	22.5	1.70	68.4%
plate 25x3x126	S175		1	CANTOR + 60%TiC	396-D-23	2306-021-04	29 June 2023	4	3.00	1.00	300	3	A	4L0	107	55	104	87	240	0.000108	0.000220	0.03	0.001	0.83	0.03	22.5	1.80	72.0%
plate 25x3x126	S175		1	CANTOR + 60%TiC	396-D-23	2306-021-05	29 June 2023	4	3.00	1.00	300	3	A	4L0	108	50	103	70	240	0.000108	0.000200	0.03	0.001	0.42	0.01	22.5	0.70	55.0%
plate 25x3x126	S500	155-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-01	26 February 2024	5	3.00	1.00	300	10	C	4L4C	108	60	96	100	240	0.000108	0.000240	0.03	0.001	1.65	0.05	22.5	3.00	48.6%
plate 25x3x126	S500	156-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-02	26 February 2024	5	3.00	1.00	300	10	C	4L2C	108	60	96	100	240	0.000108	0.000240	0.03	0.001	0.91	0.03	22.5	1.45	42.3%
plate 25x3x126	S500	157-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-03	26 February 2024	5	3.00	1.00	300	3	C	4L2C	108	60	96	100	240	0.000108	0.000240	0.03	0.001	0.91	0.03	22.5	1.48	43.5%
plate 25x3x126	S500	158-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-04	26 February 2024	5	3.00	1.00	300	3	C	4L4C	108	60	96	100	240	0.000108	0.000240	0.03	0.001	0.86	0.03	22.5	1.22	38.0%
plate 25x3x126	S500	163-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-05	27 February 2024	5	3.00	1.00	200	3	-	M2-3L2C	85	60	78	0	240	0.000108	0.000240	0.03	0.001	0.47	0.02	22.5	0.50	28.6%
plate 25x3x126	S500		1	Al14 + 60%TiC	1084-I-23	2402-008-06	27 February 2024	6	3.00	1.00	300	3	-	M2-3L2C	110	20	100	0	240	0.000108	0.000080	0.03	0.001	0.40	0.01	22.5	0.10	5.6%
plate 25x3x126	S500	170-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-07	28 February 2024	5	3.00	1.00	300	10	C	4L4C	108	40	96	100	240	0.000108	0.000160	0.03	0.001	1.04	0.03	22.5	2.00	51.2%
plate 25x3x126	S500	171-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-08	28 February 2024	5	3.00	1.00	300	10	-	M2-3L2C	85	40	78	0	240	0.000108	0.000160	0.03	0.001	0.98	0.03	22.5	1.90	51.8%
plate 25x3x126	S500	172-B-24	1	Al14 + 60%TiC	1084-I-23	2402-008-09	28 February 2024	5	3.00	1.00	300	10	-	M2-4L4C	110	60	100	0	240	0.000108	0.000240	0.03	0.001	1.41	0.05	22.5	2.30	43.4%
plate 25x3x126	AISI304	196-C-24	1	Al0 + 60%TiC	1364-N-23	2403-003-01	06 March 2024	5	3.00	1.00	300	10	A	4L0	108	40	96	100	240	0.000108	0.000160	0.03	0.001	1.25	0.04	22.5	1.70	36.3%
plate 25x3x126	AISI304	195-C-24	1	Al0 + 60%TiC	1364-N-23	2403-003-02	06 March 2024	5	3.00	1.00	300	10	C	4L4C	108	40	96	100	240	0.000108	0.000160	0.03	0.001	1.12	0.04	22.5	2.10	49.9%
plate 25x3x126	AISI304	199-C-24	1	Al0	568-E-23	2403-004-01	07 March 2024	5	3.00	1.00	300	10	C	4L4C	108	40	94	100	240	0.000108	0.000160	0.03	0.001	1.80	0.06	22.5	2.40	35.6%
plate 25x3x126	AISI304	200-C-24	1	Al0	568-E-23	2403-004-02	07 March 2024	5	3.00	1.00	300	10	C	4L4C	108	60	94	100	240	0.000108	0.000240	0.03	0.001	2.11	0.07	22.5	3.10	39.1%
plate 25x3x126	AISI304	201-C-24	1	Al0	568-E-23	2403-004-03	07 March 2024	5	3.00	1.00	300	10	A	4L0	108	40	96	100	240	0.000108	0.000160	0.03	0.001	1.29	0.04	22.5	2.50	51.9%
plate 25x3x126	AISI304	202-C-24	1	Al0	568-E-23	2403-004-04	07 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	110	40	100	0	240	0.000108	0.000160	0.03	0.001	1.36	0.05	22.5	1.80	35.4%
plate 25x3x126	AISI304	203-C-24	1	Al0	568-E-23	2403-004-05	07 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	85	40	78	0	240	0.000108	0.000160	0.03	0.001	1.35	0.05	22.5	1.70	33.6%
plate 25x3x126	AISI304	204-C-24	1	Al0	568-E-23	2403-004-06	07 March 2024	5	3.00	1.00	300	10	-	M2-3L2C	85	40	78	0	240	0.000108	0.000160	0.03	0.001	1.34	0.04	22.5	2.00	39.8%
plate 25x3x126	AISI304	205-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-01	07 March 2024	5	3.00	1.00	300	10	-	M2-3L2C	85	40	78	0	240	0.000108	0.000160	0.03	0.001	1.38	0.05	22.5	1.60	30.9%
plate 25x3x126	AISI304	206-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-02	07 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	85	40	78	0	240	0.000108	0.000160	0.03	0.001	1.26	0.04	22.5	1.50	31.7%
plate 25x3x126	AISI304	207-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-03	07 March 2024	5	3.00	1.00	300	10	A	4L0	108	40	96	100	240	0.000108	0.000160	0.03	0.001	1.20	0.04	22.5	2.10	46.8%
plate 25x3x126	AISI304	208-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-04	07 March 2024	5	3.00	1.00	300	10	C	4L4C	108	40	94	100	240	0.000108	0.000160	0.03	0.001	1.17	0.04	22.5	2.30	52.4%
plate 25x3x126	AISI304	213-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-05	11 March 2024	5	3.00	1.00	300	10	C	4L4C	108	40	94	110	240	0.000108	0.000160	0.03	0.001	1.36	0.05	22.5	2.30	45.2%
plate 25x3x126	AISI304	214-C-24	1	AlCu + 60%TiC	072-A-24	2403-005-06	11 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	110	40	100	0	240	0.000108	0.000160	0.03	0.001	1.13	0.04	22.5	1.70	40.0%
plate 25x3x126	AISI304	211-C-24	1	Al0 + 60%TiC	1364-N-23	2403-003-03	11 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	110	60	100	0	240	0.000108	0.000240	0.03	0.001	1.80	0.06	22.5	2.80	41.4%
plate 25x3x126	AISI304	212-C-24	1	Al0 + 60%TiC	1364-N-23	2403-003-04	11 March 2024	5	3.00	1.00	300	10	-	M2-4L4C	110	40	100	0	240	0.000108	0.000160	0.03	0.001	1.05	0.03	22.5	2.00	51.0%
plate 25x3x126	AISI304	226-C-24	1	AlCu + 60%TiC	072-A-24	2403-007-01	13 March 2024	5	3.00	1.00	300	3	C	4L4C	108	40	94	100	240	0.000108	0.000160	0.03	0.001	1.17	0.04	22.5	2.20	50.3%
plate 25x3x126	AISI304	227-C-24	1	AlCu + 60%TiC	072-A-24	2403-007-02	13 March 2024	5	3.00	1.00	300	3	-	M2-4L2C	110	40	100	0	240	0.000108	0.000160	0.03	0.001	1.10	0.04	22.5	2.40	58.4%
plate 25x3x126	AISI304	536-G-24	1	Al0 + 60%TiC	1364-N-23	2407-001-01	04 July 2024	5	3.00	1.00	300	3	C	4L4C	110	40	94	80	240	0.000108	0.000160	0.03	0.001	1.02	0.03	22.5	1.90	49.7%
plate 25x3x126	AISI304	537-G-24	1	Al0 + 60%TiC	1364-N-23	2407-001-02	04 July 2024	5	3.00	1.00	300	3	C	4L4C	110	60	94	80	240	0.000108	0.000240	0.03	0.001	1.87	0.06	22.5	3.70	52.9%
plate 25x3x126	AISI304	538-G-24	1	Al0 + 60%TiC	1364-N-23	2407-001-03	04 July 2024	5	3.00	1.00	300	3	C	4L4C	110	40	94	100	240	0.000108	0.000160	0.03	0.001	1.10	0.04	22.5	2.20	53.3%
plate 25x3x126	AISI304		1	Al0 + 60%TiC	1364-N-23	2407-001-04	04 July 2024	5	3.00	1.00	300	3	C	4L4C	110	60	94	100	240	0.000108	0.000240	0.03	0.001	1.65	0.05	22.5	1.30	21.1%
plate 25x3x126	AISI304	539-G-24	1	Al0 + 60%TiC	1364-N-23	2407-001-05	04 July 2024	5	3.00	1.00	300	3	C	4L4C	110	60	94	100	240	0.000108	0.000240	0.03	0.001	1.60	0.05	22.5	3.90	64.8%
plate 25x3x126	AISI304	540-G-24	1	AlMo + 60% TiC	383-E-24	2407-002-01	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	40	94	80	240	0.000108	0.000160	0.03	0.001	1.14	0.04	22.5	1.80	42.0%
plate 25x3x126	AISI304	541-G-24	1	AlMo + 60% TiC	383-E-24	2407-002-02	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	60	94	80	240	0.000108	0.000240	0.03	0.001	1.53	0.05	22.5	3.30	57.3%
plate 25x3x126	AISI304	542-G-24	1	AlMo + 60% TiC	383-E-24	2407-002-03	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	40	94	100	240	0.000108	0.000160	0.03	0.001	1.00	0.03	22.5	1.90	50.7%
plate 25x3x126	AISI304	543-G-24	1	AlMo + 60% TiC	383-E-24	2407-002-04	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	60	94	100	240	0.000108	0.000240	0.03	0.001	1.35	0.05	22.5	2.90	57.1%
plate 25x3x126	AISI304		1	AlMo + 60% TiC	383-E-24	2407-002-03	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	40	94	100	240	0.000108	0.000160	0.03	0.001	1.00	0.03	22.5	1.90	50.7%
plate 25x3x126	AISI304		1	AlMo + 60% TiC	383-E-24	2407-002-04	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	60	94	100	240	0.000108	0.000240	0.03	0.001	1.35	0.05	22.5	2.90	57.1%
plate 25x3x126	AISI304		1	AlMo + 60% TiC	383-E-24	2407-002-03	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	40	94	100	240	0.000108	0.000160	0.03	0.001	1.00	0.03	31.5	1.90	36.2%
plate 25x3x126	AISI304		1	AlMo + 60% TiC	383-E-24	2407-002-04	08 July 2024	5	3.00	1.00	300	3	A	4L4C	110	60	94	100	240	0.000108	0.000240	0.03	0.001	1.35	0.05	31.5	2.90	40.8%

Figure 17 Excel of MTS HVAF Thermal Spraying Logbook

3.2.4 SPARQL Query Example

Once the datasets are ingested, the KB can be queried using SPARQL to retrieve information that match the specific users' needs.

For example, the query shown in Figure 18 lists the property types that are associated with the coated substrate individuals, thus providing insights to the users about the content of the KB facilitating the creation of further specialised queries. In this case the output is about the TBox concepts (i.e., property types) associated with existing ABox entities (i.e., the coated substrates).

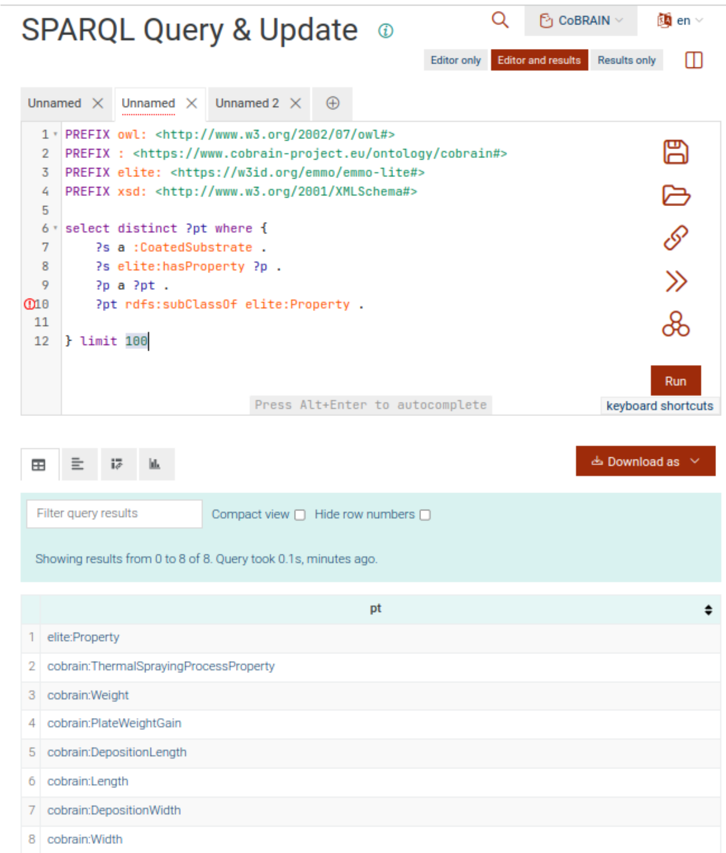


Figure 18 TBox SPARQL example.

In Figure 19 the SPARQL query is used to retrieve pairs providing information about the HVOF runs and the deposition date. In this case, the query is retrieving actual data in tabular form.

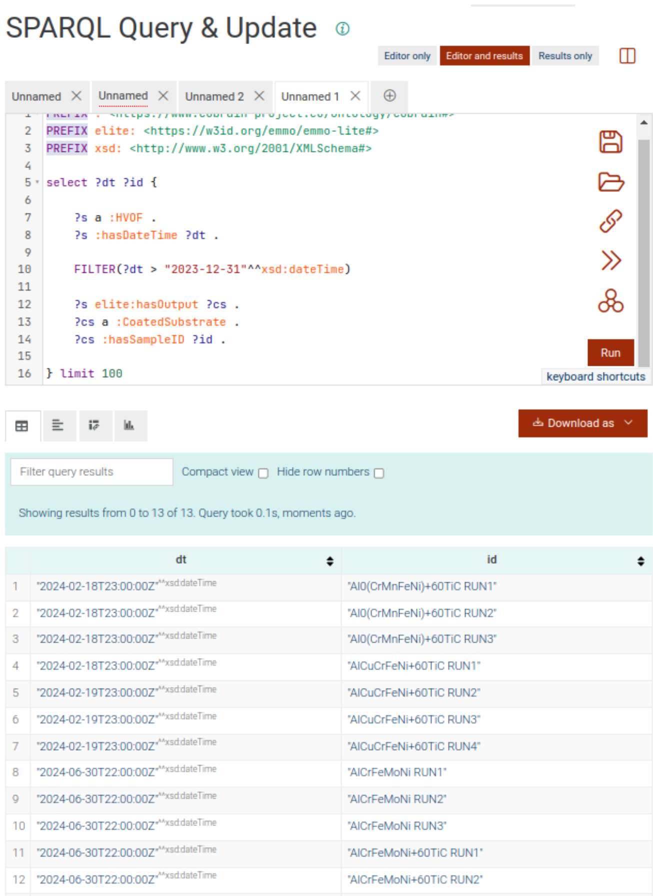


Figure 19 Data retrieval SPARQL example.

3.2.5 LLM for KB Data Retrieval

One of the latest features that commercial triplestore vendors are providing, including GraphDB, is the possibility to be queried through a LLM driven interface, as shown in Figure 20. A LLM uses the ontology annotations (e.g., labels, comments, definitions) and property relations to build SPARQL queries out of a natural language question.

This feature has been implemented into the CoBRAIN KME only for demonstration purpose, to show how semantic technologies can be used to open the door to more human friendly interfaces to large set of heterogeneous information thanks to the conceptualisation provided by an ontological framework.

What are the properties of AlCrFeMoNi+60TiC RUN3?

Here are the properties of the HVOF AlCrFeMoNi+60TiC RUN3:

- **Type**: HVOF (High Velocity Oxygen Fuel) Process
- **Label**: HVOF AlCrFeMoNi+60TiC RUN3
- **Comment**: New sample holder. Slightly unstable feed.
- **Date and Time**: 2024-06-30T22:00:00Z
- **Run Number**: 1
- **Sample ID**: AlCrFeMoNi+60TiC RUN3
- **Input**: References powder or material used in the process.
- **Output**: References the resulting sample from the process.
- **Various Relationships**: It has several semiotic and mereological relationships to other entities.

can you list the properties of the powder?

The properties of the powder used for the SAMPLE AlCrFeMoNi+60TiC RUN3 include:

- **Type**: Coated Substrate, Object, System, Resource
- **Label**: SAMPLE AlCrFeMoNi+60TiC RUN3
- **Run ID**: AlCrFeMoNi+60TiC RUN3
- **Relationship**: Related to the HVOF AlCrFeMoNi+60TiC RUN3 process
- **Has Component**: References specific components of the powder
- **Various Semiotic Relationships**: Includes related signs, outputs, and mereological relationships

List the HVOF processes that have a spraying efficiency with a data value higher than 55%

Here are the HVOF processes that have a spraying efficiency with a data value higher than 55%:

1. **HVOF Cantor RUN4**: 64.42%
2. **HVOF Cantor+60TiC RUN2**: 60.79%
3. **HVOF Cantor+60TiC RUN3**: 58.33%
4. **HVOF Al0(CrMnFeNi) RUN1**: 60.97%
5. **HVOF Al0(CrMnFeNi) RUN2**: 59.40%
6. **HVOF Al0(CrMnFeNi) RUN3**: 56.73%
7. **HVOF Al14(CrMnFeNi)+60TiC RUN1**: 64.13%
8. **HVOF Al14(CrMnFeNi)+60TiC RUN3**: 56.06%
9. **HVOF Al10(CrMnFeNi) RUN1**: 59.72%
10. **HVOF Al10(CrMnFeNi) RUN2**: 57.48%
11. **HVOF Al10(CrMnFeNi) RUN3**: 56.52%
12. **HVOF Al14(CrMnFeNi)+60TiC RUN4**: 57.12%
13. **HVOF Al0(CrMnFeNi)+60TiC RUN1**: 59.81%
14. **HVOF Al0(CrMnFeNi)+60TiC RUN2**: 58.72%
15. **HVOF Al0(CrMnFeNi)+60TiC RUN3**: 55.58%
16. **HVOF AlCuCrFeNi+60TiC RUN1**: 59.87%
17. **HVOF AlCuCrFeNi+60TiC RUN2**: 56.86%
18. **HVOF AlCuCrFeNi+60TiC RUN3**: 55.06%
19. **HVOF AlCuCrFeNi+60TiC RUN4**: 60.45%
20. **HVOF AlCrFeMoNi+60TiC RUN1**: 61.03%
21. **HVOF AlCrFeMoNi+60TiC RUN3**: 58.97%

Figure 20 LLM based query examples.

4 Conclusions – Next Actions

This deliverable presents an overview of the CoBRAIN Knowledge Management Environment, and its implementation through a Knowledge Base built upon the GraphDB triplestore commercial solution.

An initial batch of datasets from MBN, UMR and ACCESS have been mapped and uploaded to the KB, while the full set of CoBRAIN datasets will be mapped and uploaded during the next part of the CoBRAIN project as soon as data will be made available by the partners.

The CoBRAIN ontology will be further updated to include specific concepts (classes and relations) that will be required by each simulation, characterisation of experimental user case scenario, and according to the datasets that will be provided by partners.

The SPARQL endpoint for the CoBRAIN KB is exposed on a public IP, hosted by UNIBO, ready for accessibility to the public. Access criteria, domain name redirection, and public announcement will be provided via the consortium dissemination channels after the M24 meeting.

5 Attainment of Objectives

Table 1 - General project objectives related to WP1 and their status on M24.

Ref.[4]	General Objective	Status
O2.1	Knowledge base repository for the ontological representation of Thermal Spray	TBox completed. ABox and data linking at M24.

Table 2 - Specific objectives of WP1 and their status on M24.

Ref.[5]	Work Package Objective	Status
WP1.1	to Specify the complete MODA and CHADA to be used in the project.	Done with D1.2 and D1.3 at M06.
WP1.2	to Create a set of ontological relations that connect and describe Modelling, Characterization and TS Processes.	Done with D1.1 at M12 through the CoBRAIN ontology and the EMMO framework. To be expanded up to the end of the project M48 according to project needs.
WP1.3	to Create an OWL-DL ontological representation of the manufacturing processes.	Done with D1.1 at M12.
WP1.4	to Store everything in a Knowledge Base repository exploiting commercially available RDF Triplestore.	Done with D1.4 at M24 to be concluded for all CoBRAIN shared data at M48

[4] Reference to the general project objectives stated from page 4 of Part B of the Annex 1 – Description of Action

[5] Reference to the specific objectives of the workpackage as listed in Part A of Annex 2 – Description of Action