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**DEVELOPMENT OF A MANUFACTURING ONTOLOGY FOR FUNCTIONALLY
GRADED MATERIALS**

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ABSTRACT

The development of manufacturing technologies for new materials involves the generation of a large and continually evolving volume of information. The analysis, integration and management of such large volumes of data, typically stored in multiple independently developed databases, creates significant challenges for practitioners. There is a critical need especially for open-sharing of data pertaining to engineering design which together with effective decision support tools can enable innovation.

We believe that ontology applied to engineering (OE) represents a viable strategy for the alignment, reconciliation and integration of diverse and disparate data. The scope of OE includes: consistent capture of knowledge pertaining to the types of entities involved; facilitation of cooperation among diverse group of experts; more effective ongoing curation, and update of manufacturing data; collaborative design and knowledge reuse.

As an illustrative case study we propose an ontology focused

on the representation of composite materials focusing in particular on the class of 'Functionally Graded Materials' (FGM) in particular. The scope of the ontology is to provide information about the components of such materials, the manufacturing processes involved in creation, and diversity of application hanging from additive manufacturing restorative dentistry. The ontology is developed using Basic Formal Ontology (BFO) and parts of the Ontology for Biomedical Investigation (OBI).

NOMENCLATURE

BFO Basic Formal Ontology
ERP Enterprise Resource Planning system
FGM Functionally Graded Materials
OBI Ontology for Biomedical Investigations
OE Ontology Engineering
MIG Metal Inert Gas welding
PDM Product Data Management system
PLM Product Lifecycle Management system

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INTRODUCTION

Information management encompassing the lifecycle of acquisition, curation and dissemination of material data have posed significant challenges in both academic and industrial domains. Over the years, relevant communities have accumulated ever larger amount of scientific data, and this accumulation has created a shortfall in effective information management. Improving this effectiveness is the key to obtaining better results in both research and development.

Typically, data about materials science and engineering relates to four elements: composition of the material produced, properties of these materials, processing, performance in finished products [1, 2].

Oftentimes materials science data, of the sorts analysed by the scientists, are stored in multiple, autonomous, distributed, and heterogeneous sources, codified in different, and in many cases incompatible, formats often in the form of raw data obtained from lab instruments acquisition and or from measures of performance of basic properties, like corrosion data or fatigue data.

A less discussed (but perhaps more critical) challenge is the semantic inconsistency of explicit and shared information as between different users and different applications [3, 4]. Different aspects of this problem have to be considered, including: different ways of classification of materials due to different scopes, semantic discrepancy of synonyms and homonyms, different representation of similar data. Further comprehending this matter is the fact that the inherent task of classification of materials is very complicated. For example, asking a query concerning a corrosion resistant material over multiple data sources often does not result in the right answer because of lack of proper consistent classification of the information or because of lack of knowledge of the appropriate terms which would need to be used in the query. To address these problem requires a better data management infrastructure of a sort, which can facilitate the process of resolving semantic heterogeneity and give to the users a unified view of distributed data sources using consensus terms that they can easily understand.

To explore the little ideas better, we consider the illustrative case study of a subclass of materials - Functionally Graded Materials. FGM not only reflect the complexity and heterogeneity of scientific data and information, but have taken a special importance in a range of applications.

Functionally Graded Materials

During all of human history, scientists and technologists have sought to overcome the problems caused by poor characteristics of pure metals by combining them in alloys, where one

metal is mixed in solution with another metal or non-metal substance in order to obtain a new material with better characteristics. Some of the limitations of alloying techniques are related to the maximum quantity that can be dissolved in a solution, due to thermodynamic equilibrium limits or difficulty in alloying two dissimilar materials [5, 6].

Powdered Metallurgy (PM) based techniques represent a alternative methods used to overcome some of the problems associated with conventional alloying. However they bring other disadvantages, such as poor strength with resultant limitations in shapes that can be generated [7].

Composite materials are a class of advanced materials, characterized by two or more materials, usually having different physical and chemical properties, combined in solid states. Composite materials provide properties that are different from the individual parent materials. They are manufactured by using a process called delamination which involves separation of fibers (that are synthetic substances significantly longer than wide) from the matrix [8]. These materials can be extremely strong, bearing huge load forces, but they present limitations when working in high temperatures, as when, for example, two metals have different expansion coefficients.

Functionally Graded Materials (FGM) are a subcategory of composite materials in which the properties can vary over spatial coordinates [9, 10]. Figure 2 illustrates multiple particles of two different materials A and B mixed together following a specific for the mixing gradient as a mathematical function depending only on the vertical direction. Thus, sharp interfaces between fibers are replaced by gradient interfaces, producing smooth transition between the two components.

FGM can be fabricated in different ways, depending on the desired shape. Fabrication can be of bulk volumes of material or of thin coatings: the former are typically produced powder metallurgy based techniques, centrifugal casting methods, or solid freeform technology. The latter typically involve vapor deposition, spraying, and so on. FGMs are used in many areas of application including aerospace, automobile, medicine, sporting equipment, energy, sensors and optoelectronics. A significant amount of research is aimed at improving the fabrication processing and properties of the FGM. For that reason there is the need to adopt methodologies and specific tools that enable the storage and management of data about FGMs to enable the sharing and discovery of these data among materials scientists and by manufacturing engineers. In this paper is presented an application of Ontology Engineering (OE) to the description of manufacturing tasks, fabrication processes, mechanical and physical parameters, composition and scopes of FGMs with the goal of promoting sharing and discoverability of FGM data.



Figure 1: FGM Scheme [11]: • particle of material A, ◦ particle of material B

Ontology in Manufacturing and Industrial Engineering

Ontology originated as the philosophical study of the nature of beings. Nowadays ontology is used in computing and related fields to study the types or categories of existent entities in reality and the relations between these types with a view to providing controlled vocabularies for describing data [12]. OE is the application of this methodology to the engineering field. The methodology allows the formulation of a vocabulary relative to a specific field, definition of terms in this vocabulary at different levels of formality, and the formal specification of relations between these terms. In practice the development of such a structure includes: the definition of classes of entities, taxonomic arrangement of class hierarchies (including sub- and super-classes), provision of examples of instances of the identified classes, and input/edit parameters creation of tags or annotations to corresponding data.

Multiple studies of OE applied to industrial engineering can be found in the literature. In many of these ones the main scopes regarded the development of common languages for the collaboration between different domains in the same or different academic/industrial entity. Different ontological tools have been developed in the field of manufacturing to model manufacturing systems and performing of their configuration, simulation, retrieve, reuse and management of data for design. Shortfalls in interoperability can be rectified by improving collaboration among experts in design and management, by promoting the use of common terms and definitions and the sharing of common representation of data through standard interfaces. [13] describes a holistic model representing manufacturing systems based on the ANSI/ISA95 international standard, defined for the development of automated interfaces between enterprises and control systems. This system is built using the Process Specification Language (PSL), an ontology that provides a way to formally describe a process and its characteristics. With the help of PSL standard is possible to develop robust and reliable framework to formalize knowledge related to a process, with a high level of interoperability standard. However this standard is still not widely

adopted in the industrial domain, probably because of the perceived complexity at the enterprise level. The goal of [13] was to model manufacturing line structure able to support numerical simulations showing how, with the aid of the ontology, it is possible to select process types and retrieve descriptions, resources and machines for a specific manufacturing process. The results suggest that with the help of PSL it is possible to develop a robust and reliable framework to formalize knowledge related to processes of this sort, with a high level of interoperability. PSL is however still poorly adopted in the industrial domain, probably because of its perceived complexity at the enterprise level.

The same needs of collaborative design and knowledge reuse led the authors of [14] to develop an ontological framework, for specifying the terminology used in the field of manufacturing design. They pre-identified a roadmap for the development of the ontology including the definition of classes, arrangement of these in taxonomic hierarchy, subclasses, and superclasses, definition of properties and specification of allowed values, creating instances of classes, and input/edit values of their properties. The roadmap is composed by the following steps:

1. Determine the domain and scope of the ontology
2. Consider reusing existing ontologies
3. Enumerate important terms in the ontology
4. Define the classes and the class hierarchy
5. Define the properties of classes
6. Define the facets of the slots
7. Create instances

On this basis the authors were able to sketch a mid-level ontology relating to design for manufacturing, including definitions of principal classes such as *manufactured products*, *manufacturing features*, *manufacturing processes*, and so on. The study case is related to the analysis of costs involved in Metal Inert Gas welding processes (MIG), feasibility and accessibility analysis of filler material and machine selection. The authors also provide accompanying decision support tool with a local and online versions.

In [15] the authors list projects in which ontology is used as a tool for assessment of resources and management of information in product lifecycle management. For example in the European Union funded project called "Linked Design" (<http://www.linkeddesign.eu/>), the aim is to develop an integrated ontology based platform for manufacturing design that federates all relevant product lifecycle information independent of format, location, originator, and time. The use cases are mainly referred to the proposal and operational phase of a product lifecycle; the goal of the platform is to have an automated system to calculate the Life Cycle Costs (LCC) of the operation of a production line and to optimize the line configuration according to these costs including environmental impact. In the Virtual Factory Framework project (<http://www.ims.org/2011/>

11/vff-virtual-factory-framework/) the aim is to develop an integrated collaborative virtual ontology based environment for facilitating the sharing of resources, manufacturing information, support of design and management of all entities involved in the workings of a factory, in all phases of the factory lifecycles. The framework is characterized by a module for the visualization of the factory layout and by a module for the design and evaluation of performance of product lines.

Another example of use of ontology in industrial engineering is analyzed in [16]. The petroleum industry is characterized by specialized companies and complex operational structures, resulting in the development of multiple terminological standards in recent years. These standards provide support for interoperability within the particular disciplines on which are based, but they impede effective collaboration across disciplines and organizational borders. Referring to the Integrated Information Platform project, the authors discuss the results of a developed and formalized OWL ontology for the Norwegian petroleum business. The ontology is used in the automated production of reports, and is shown to represent a step towards semantic interoperability and towards integrated operation of oil industry plant in Norway.

The ontology developed for the present study has been created with Protégé ontology editing software <http://protege.stanford.edu/>. Protégé makes it possible to represent definitions of terms and relations in ontologies and enables reasoner-based checking for ontology consistency. The resulting ontology is an easily configurable open source tool for describing data in FGM domain.

This article will summarize our efforts on development of the ontology of the case of the FGM, starting by the considerations about the Upper Level, the mid and domain level and finally example of information retrieval of material data using this framework.

DEVELOPMENT OF THE ONTOLOGY

In the previous section, we outlined a number of few publications about relating to the use of OE in industrial engineering. Some of the common aspects related to each article can be summarized as follows:

1. Ontology supporto for cooperation among experts in different fields
2. Consistent management and update of manufacturing data
3. Collaborative design and reuse of existing data and information
4. Capturing of definition terms and relations
5. Enabling discoverability of data in web-based environments

The standard tools for data management available in the market include Product Lifecycle Management (PLM) and

Table 1: Scheme of the ontology development

Upper Level	Mid Level	Domain Level
BFO	OBI & Manufacturing Literature	FGM literature

Product Data Management (PDM) systems, Enterprise Resource Planning (ERP) systems. PLM systems are used for data integration of processes, business systems and, ultimately, people in an extended enterprise. With a PLM software is possible to manage efficiently this information during the entire lifecycle of a product and effectively track the relative costs from conceptualization, design and manufacture, through service and disposal (http://www.plm.automation.siemens.com/en_us/plm/). PDM systems permit to manage product and process data and information in a single, central system. This information includes computer-aided design data, models, parts information, manufacturing instructions, requirements, notes and documents. A PDM system is ideally accessible by multiple applications and multiple teams across an organization (http://www.plm.automation.siemens.com/en_us/plm/pdm.shtml). ERP systems represent a category of business-management softwares that enable an organization to collect, store, manage and interpret data from many business activities like product planning and cost, manufacturing or service delivery, marketing and sales, inventory management, shipping and payment.

An ontology framework based on OE could be adopted for the same scopes in both academic and industrial research fields. An ontology could be open, free and shareable among experts, although these techniques are in early development for the industrial field. The ontological structure described in this study is articulated as shown in Table 1.

The ontology can be analyzed by three different levels of complexity; the upper level is described adopting the classes defined by Basic Formal Ontology (BFO) [17]. The mid level is developed using some of the classes belonging to Ontology for Biomedical Investigation (OBI) [18] and further knowledge about manufacturing of material retrieved in literature.

This structure is created in order to store, share and retrieve information about FGM by means of more or less complex query questions like select which of FGM can be used in constructions having particular properties satisfying certain values or certain ranges.

Use of BFO as upper level ontology

BFO in the release 2.0 http://ncorwiki.buffalo.edu/index.php/Basic_Forma Ontology_2.0 is an

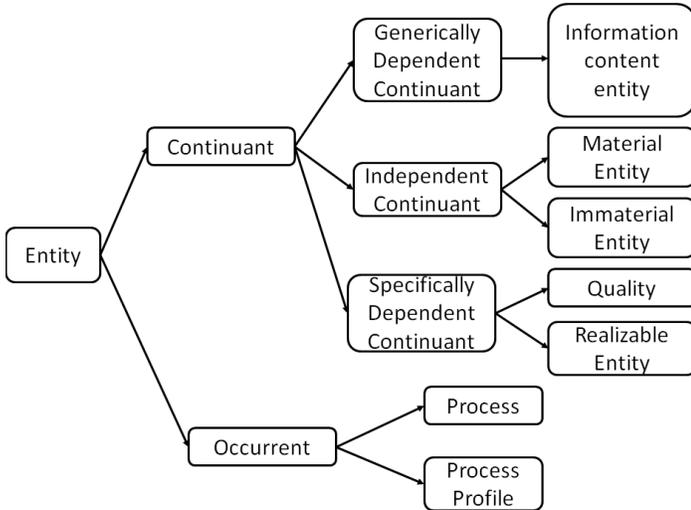


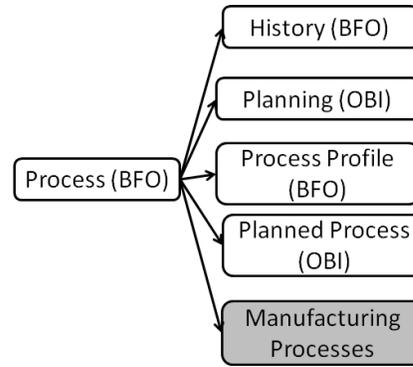
Figure 2: Basic Formal Ontology Classes [19]

upper level description of entities that assist the developer on the organization and integration of different types of information [19]. BFO describes entities in terms of *Occurrent* and *Continuant* (Fig. ??). A *Continuant* is an entity that exist through time while maintaining its identity, such as object, qualities and functions. *Continuant* is contrasted with *Occurrent* that are events of happenings in which continuants participate, like *Process*.

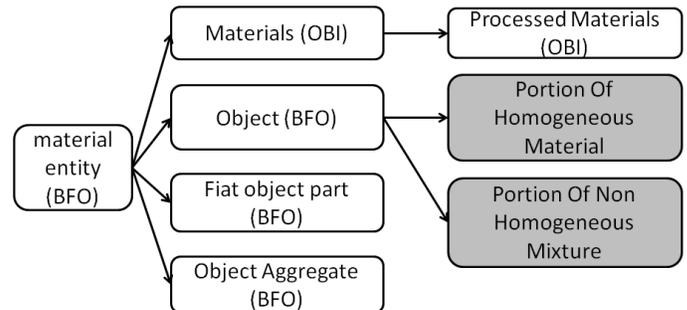
The most important subclass of *Continuant* is *Material Entity*, that includes some portion of matter as part. In this study, materials are considered as portion of material entity characterized by molecules or atoms.

Another important class of BFO is *Realizable Entity*, which include *Role* and *Function* [17]. These are subclasses of *Specifically Dependent Continuant*: that means that their existence depends on a *Independent Continuant (Material Entity)* and that are associated to certain kinds of processes or activities that can be realized. *Role* is a class that identifies realizable entity: it exists because of some quality bearer, like a material entity. In this study, *Role* is used to describe how the components of a composite material or FGM, are participating in material structure. *Function* is a disposition that exists because of the bearers physical make-up that is something the bearer possesses because it came into being. In the actual study this class is used to describe particular scopes and applications of the different portions of material.

Quality is a *Specifically Dependent Continuant* that does not require any further process in order to be realized. Here is used to describe particular parameters of portions of material, such as physical qualities deriving from a specific manufacturing process.



(a) *Material Entity* class and subclasses



(b) *Process* class and subclasses

Figure 3: Ontology Mid Level Classes

Development of the mid level and domain ontology

The ontology under creation has been developed taking care about the four critical aspects noted in [1, 2]:

1. Composition
2. Properties
3. Processing
4. Performance

The mid level ontology has been developed by considering part of the classes available in the OBI and information on literature about manufacturing of materials. OBI <http://purl.obolibrary.org/obo/obi.owl> is an ontology that provides resourced to represent biomedical investigation [18]. The description of experiments typically is an activity that does not follows specific standard terminology, creating problems in the comparison of results, reproduction and analysis. OBI can be applied to different biomedical investigations, in order to improve the understanding of experimental process and increase processing and integration within the Semantic Web. OBI is useful to understand how materials, processes related to materials and scope of the analysis are represented in an ontological framework. Some of the reused classes are represented in Fig. 3.

Fig. 3a shows the representation of the hierarchy of *Process* defined by BFO and OBI. In the grey box is represented the

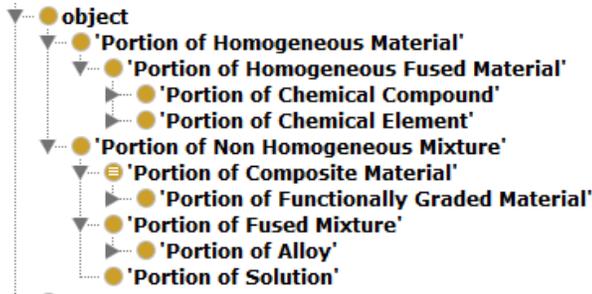


Figure 4: Object class taxonomy



Figure 5: Material Quality taxonomy

subclass *Manufacturing Process* that considers all the processes to fabricate materials. Fig.3b shows the taxonomy of the class *Material Entity*. The classes in the greyboxes have been added to consider the different kind of portions of material: *Portion of Homogeneous Material* represents the set of portions characterized by one uniform type of portion of material while the class *Portion of Non Homogeneous Mixture* represents portions that are mixture of other portions of material. The taxonomy of the class *Object* edited in Protégé is shown in Fig. 4.

Portion of Chemical Compound is defined "Any substance consisting of two or more different types of atoms (chemical elements) in a fixed proportion of its atoms (i.e., stoichiometry) can be termed a chemical compound; the concept is most readily understood when considering pure chemical substances" [20]. *Portion of Chemical Element* is defined as "a chemical element or element is a chemical substance consisting of atoms having the same number of protons in their atomic nuclei" [21]. *Portion of Composite Material* is defined as a portion of material made from two or more constituent materials with significantly different physical or chemical properties. Such combination results in a material with characteristics different from the individual components. The individual components remain separate and distinct within the finished structure. The new material may be preferred for many reasons: it could be stronger, lighter, or less expensive when compared to traditional materials" [22]; *Portion of Functionally Graded Material* is defined as "composite material characterized by two or more constituent phases. Main characteristics are continuously variable composition and mono-directional/bi-directional/tri-directional gradients of composition." [11]. In the class *Portion of Fused Mixture* is possible to find *Portion of Alloy* that is "mixture of metals or a mixture of a metal and another element, defined by metallic bonding character. Alloys may be a solid solution of metal elements (a single phase) or a mixture of metallic phases (two or more solutions)" [23].

A taxonomy about quality of materials has been developed to identify specific properties involved in the description of material and relative processes. Some of the main mechanical and chemical properties characterizing main FGM literature are resumed in Fig. 5.



(a) Component Multiplicity taxonomy



(b) Process Quality taxonomy



(c) Gradient Quality taxonomy

Figure 6: FGM quality taxonomy

Fig. 6 lists the considered properties related to FGM: *FGM Component Multiplicity* indicates the quantity of different components that are present in the FGM portion of material (Fig. 6a); *FGM Process Quality* and its subclasses describe the properties of a particular processes for FGM forming [11] (Fig. 6b); *Gradient Quality* describe any quality related to the shape, mathematical function, continuum of the gradient of the material (Fig. 6c). The subclass *Gradient Directionality* describes the type mathematical function that characterizes the mixing gradient. With reference to the number of independent variables, the gradient could be: monodirectional (one variable), bidirectional (two variables), tridirectional (three variables). In [24] the authors even defined the possible typologies of gradients in relation with its nature: *Gradient Size Multiphase*, *Porosity Gradient*, *Single Phase Chemical Composition Gradient*.

The various applications of FGM has been considered as subclass of *Disposition*. About the medical field, an important disposition for biomedical application is *Biocompatibility*, that



Figure 7: Processes taxonomy

refers to the ability of a biomaterial to perform its desired function with respect to a medical therapy, without eliciting any undesirable local or systemic effects in the recipient or beneficiary of that therapy, but generating the most appropriate beneficial cellular or tissue response in that specific situation, and optimising the clinically relevant performance of that therapy [25, 26].

All the manufacturing processes are inferred by literature about FGM. These were formalized in the taxonomy of Fig. 7 [11, 24, 27, 28]. *Composites Material Fabrication* and *Functionally Graded Material Forming* represent the classes of manufacturing processes considered in this study. FGM fabrication processes mostly belong to three main categories of processes: *Melting Process*, *Polymer Based Process* and *Deposition Process* that contains the main subclasses *Powder Metallurgy Based Process* and *Coating Deposition Process*.

In Fig. 8 is represented the proposal taxonomy of the different kind of application for FGM [5, 27, 28]. All these classes of application are defined on extraction and consideration the available literature.

Examples of classification of FGM in the ontology

The FGM classes has been added semantically to the framework using relations. The relations in the ontology are used to create axioms: *isAppliedTo* is a relation that connects each portion of material (domain) to each specific field of application (range). *isManufacturedBy* relates each portion of material (domain) with a manufacturing process (range). *isConstituentOf* is necessary to associate portions chemical elements or chemical compounds with a specific FGM. *hasGradientTypology* is used to describe the type of gradient characterizing the material under exam and *hasBiocompatibility* obviously is indicating the possibility for a type of material to be used for biomedical applications.

The first example of FGM considered in the ontology is a polyethylene based polymer (Fig. 9) [28]. This artificial biomaterial is used for knee joint replacement and shoulder replacement (Fig. 9c) has been developed by building a graded structure consisting of fibre reinforced high-density polyethylene (HDPE) combined with a surface of UHMWPE (Fig. 9b) and it is characterized by a single phase chemical composition gradient (Fig. 9d). With the addition of this information to the framework is possible to compute qualitative queries about the different kind of materials used for knee replacement or shoulder replacement

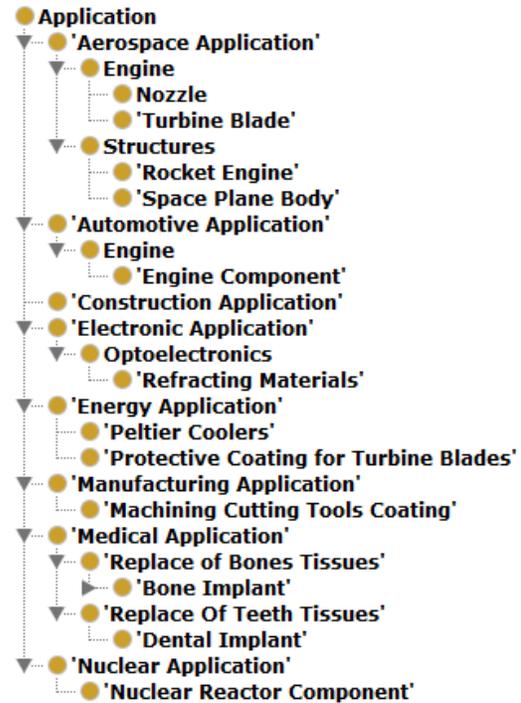


Figure 8: Application Taxonomy

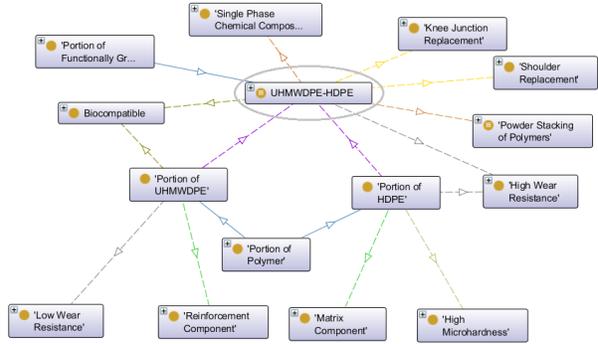
or asking for materials that satisfy precise mechanical resistance requirements.

The composite Titanium-Vanadium-Aluminum (Fig. 10) is an FGM applied to Dental implants (Fig. 10b). It's characterized by a porous gradient and is obtained by selective laser sintering process (Fig. 10c). Referring to [29], the authors describe one individual of the this class of FGM, whose name is Ti-6Al-4V (Fig. 10c) and the composition is 90.08 % Titanium, 5.67 % Aluminum and 4.25 % Vanadium. One of the mechanical properties tested in the experiments is the Young Modulus, whose value reaches 104 GPa in the compact titanium side of the portion of material, 77 GPa is measured in the porous side of the portion of material.

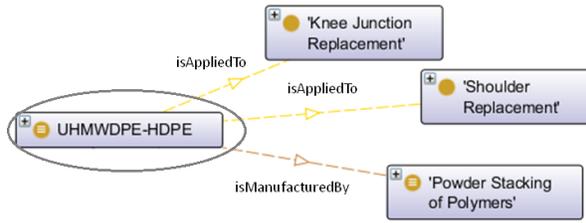
Semantic Queries about FGM materials The software Protégé facilitates placing of queries on the system, reasoning about them and inferring one presenting answers back to the user. Hermit 1.3.8.3 (<http://www.hermit-reasoner.com/>) has been used as a convenient reasoner while DL Query serves as the query tool.

A first sample query about the ontological framework is the research of a FGM able to be used in *Knee Junction Replacement* or *Shoulder Replacement*, obviously biocompatible. The syntax correspondent syntax is

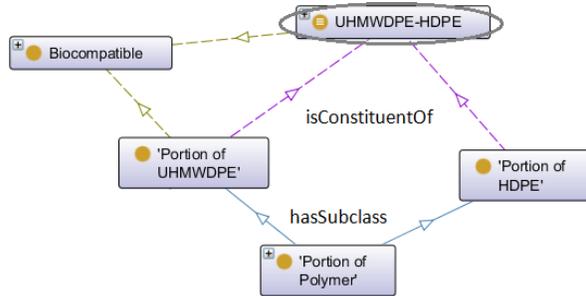
'Portion of Material' and (hasBiocompatibility some Bio-



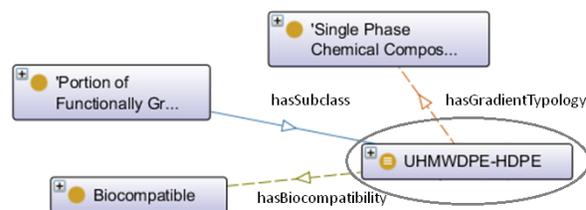
(a) FGM classes and relations



(b) FGM Constituents



(c) Applications and forming processes



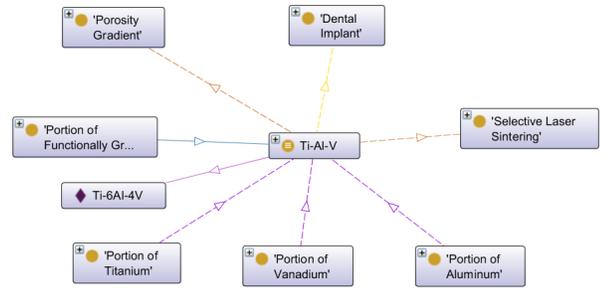
(d) Gradient and biocompatibility

Figure 9: UHMWDPE-HDPE scheme

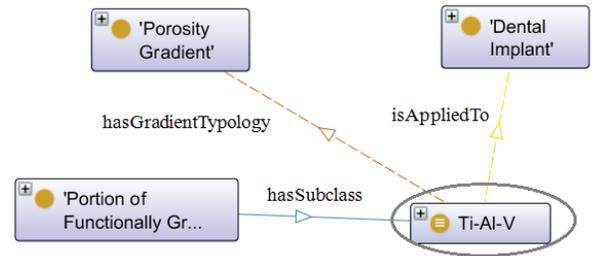
compatible) and (*isAppliedTo* some ('Knee Junction Replacement' or 'Shoulder Replacement'))

the answer to that syntax, in accordance to the experience described in this article is obviously UHMWDPE-HDPE.

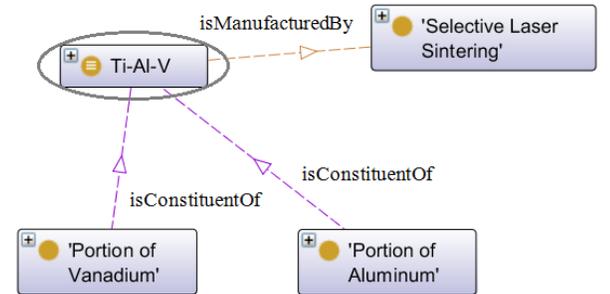
Another query sample is asked about the research of a material having high wear resistance. The syntax is as following



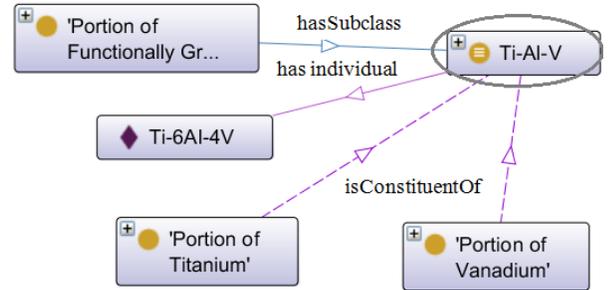
(a) FGM classes and relations



(b) Applications and gradient



(c) Constituents and processes



(d) FGM constituents and individuals

Figure 10: Ti-Al-V scheme

'Portion of Material' and (*hasConstituent* some 'Portion of Polymer') and *hasMaterialWear* some 'High Wear Resistance'

The answer corresponds to UHMWDPE-HDPE. The previous query examples has been formulated with respect to object prop-

erties of the ontology. The next sample query is about data property, asking for a material with precise response to a mechanical property. Specifically is requested a material that can be used for dental implants having young modulus higher than 100 GPa. The question is referred to the porous material based on titanium, aluminum and vanadium. The syntax is:

'Portion of Material' and isAppliedTo some 'Dental Implant' and hasCompactYoungModulus some integer [$i=100000$]

CONCLUSIONS

Our work has focused on developing the fundamentals of an ontology framework for storing and sharing material data. Complex activities related to the experimentation and discovery of new materials, such a composite materials of FGM, often presents lack of standardization. Hence an ontology to serve as an open and shareable tool that permits to the experts to add, manage and retrieve new data about new materials can significantly enhance the efficiency of the research. Specifically, we focused attention on formalization of the classes related to the information about functionally graded materials. Aspects about compositions, application, processes and characteristics have been mainly considered. Materials, applied to medical and dental fields, have been described and added to the framework using existing superclasses and relations. Subsequently it became possible to query the system to retrieve specific information about the materials, their applications, experimental results. The next steps include the enrichment of the ontology with more classes of materials and possibly more individuals of the classes in order to make the ontology applicable to real cases and permitting the release of the framework.

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