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Analysis of the applicability of domain ontology in copper alloys processing

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Abstract

Efficient use of corporate resources in the form of intellectual capital is due in large measure to effectiveness of knowledge codification and distribution systems. Making intellectual resources available to employees in time short enough to enable efficient use is possible due to search tools. The goal is to provide relevant and significant knowledge in right time. Full-text search in the databases, whether the use of directories, no longer fulfills its tasks in a situation where knowledge comes from diverse, often semantically and formally inconsistent sources. The creation of an ontology-based system would eliminate these difficulties. This paper proposes algorithms of development domain ontology of the knowledge of copper alloys, and also analyzes the feasibility of such a system. The estimate benefits of implementation, according to the authors, as well as the main difficulties associated with implementation was presented. Conclusions reached are the basis for a broader study on the feasibility of this class of systems in the foundry industry. Anticipated solution of this problem oriented on the processing of copper alloys, information-share tools discussed in the article must include specific to foundry processes issues, and thus will have an innovative character.

Keywords: Application of Information Technology to the Foundry Industry, Ontologies, Knowledge Integration, Copper Alloys, Knowledge Codification

1. Introduction

Supervisory computer systems controlling specific production tasks or supporting human decisions need to use, like people, scientific and technical knowledge that is available for them in the appropriate form. The creation of a knowledge-based computer system requires the processing of the classical forms of knowledge into system representation knowledge. As classic forms of knowledge we consider the studies in the literature, standards and technical manuals. Depending on the nature of knowledge representing the domain, an appropriate formalism, which will reflect the best its characteristics should be chosen.

There are many ways to formalize scientific and technological knowledge [1]. One of the oldest is to create mathematical models to describe the processes, events or objects using mathematical expressions. However, there is a number of problems for which the classical approach is inadequate. The undoubted advantage of mathematical models is the case of implementing them in computer systems. However, the mathematical description of the real world has a limited applicability. While it is not very difficult to describe with this convention the heat exchange or diffusion process, it is quite impossible to write down, using a mathematical expression the heat treatment procedures for the selected item.

The authors discern the need of integration of distributed knowledge in the field of processing non-ferrous metals and their alloys. In the foundries as well as other enterprises and institutes series of studies are conducted aimed at production of machines parts with the best properties. Scientists, technology experts in the domain benefit from many sources of scientific knowledge and technology. The results of experiments conducted by them are also valuable sources of information and knowledge. A characteristic feature of this knowledge is the heterogeneity of forms and various criteria for ordering it. Extraction of knowledge needed to solve a specific problem, such as a selection of appropriate heat treatment parameters to achieve desired mechanical properties, requires a tremendous amount of work, usually a large group of people. Organizing this knowledge by a clear key and the possibility of automatic processing and complement greatly facilitates their access to certain areas.

Analyzing knowledge of materials, with particular emphasis on areas related to the bronze foundry alloys has highlighted the hierarchical system of its key concepts, in which the concept situated below inherit the characteristics (attributes) of an overarching concepts. These attributes often differ only in values.

Figures 1 and 2 shows a hierarchical way to organize pieces of knowledge about metals and their alloys.

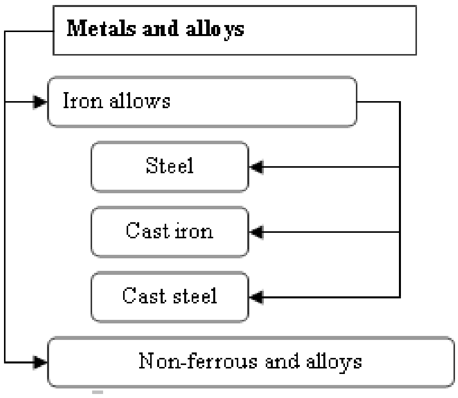

Fig. 1. Hierarchical structure of knowledge about alloys

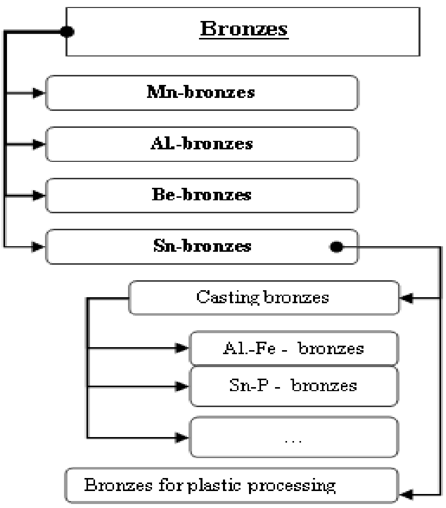

Fig. 2. Hierarchy of bronzes

One of the established formalisms rapidly developing in recent times and perfectly reflecting the character of described area is ontology. Literature gives many definitions and examples of applications of this formalism [2, 3]. An ontology is a logical representation of domain knowledge and relation between objects existing in it. It differs from other ways of representing knowledge, not only providing a scheme or the description of the domain, but with tools of logic (axioms, definitions, rules) allows us to describe the hierarchy of its components and criteria for their classification. Construction of ontologies is based on the frames, can use several types of frames: classes, slots, facets, instances. Each frames will be presented on the example of domain ontology described in Chapter 2

2. Domain ontology

Classes are defined as sets of concepts. Ontology consists of three basic classes: *elements, materials* and *processes*. Each class has its own hierarchy which is a representation of the basic concepts in a given range. Part of ontology of the material, noted using the Protégé 3.4 editor [4] is shown in Figure 3.

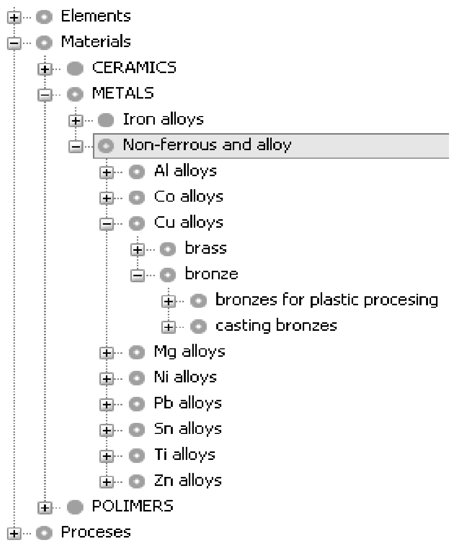

Fig. 3. The structure of hierarchy of the MATERIALS class

Slots hold certain properties and characteristics of objects from the class. Sometimes are called the *roles* because of the dynamic changeability of object properties. Slots can have different **facets** (imposed constraints) describing: the allowed types of value (e.g. *Boolean, String, Class, Float, Instances, Integer, Symbol, Any*), allowed values (e.g. max and min) and the number of values - cardinality which defines how many values the slot can have. One of slots (features/attributes) characterizing the concept of *bronzes* is the content of Cu element. At the level of abstract class called *bronzes* we have to impose some limitation related to its contents max. 80-90% wt. Fragment of the hierarchy and attributes view (slots) and their restrictions (facets) assigned for the *bronzes* class are shown in Fig. 4 and 5.

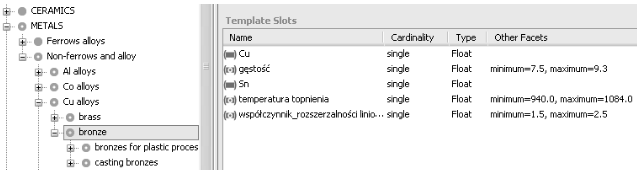

Fig. 4. The slots and facets of the *bronze* class

Fig. 5. Ontological hierarchy of *casting_bronzes* class

The various subclasses inherit the characteristics of the parent class but other restrictions can be imposed on each of them in the form of **facets**. In addition to slots of the inherited subclasses may have their own individual characteristics, and so subclass called *aluminum-iron-manganese bronzes* can be characterized by additional attributes: the contents of Al, Mn, Fe, which are imposed facets - Figure 6.

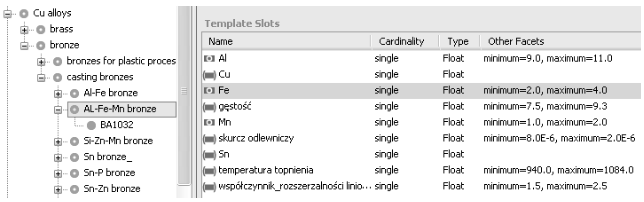

Fig. 6. Facets imposed on class *aluminum-iron-manganese bronzes*

Instances are the objects of a defined class, for example, an instance of tempering (which is a subclass of the process) has defined specific values of attributes characterizing it. For example, the instance called *tempering_H1* (temperature: 950°C, cooling_medium: water) – Figure 7.

Fig. 7. Instances of subclass *tempering*

3. Database-ontology mapping

3.1. Database for the experiment

Analysis is based on the results of tests carried out on four heats of bronze BA1032 (E, F, G, K) under various types of modification (heat E - without modifying, F - modified calcium [Ca], G - modified potassium [K], heat F – modified boron [CuB_2]). For total the results for 60 samples were taken under analysis.

Individual samples were subjected to different types of heat treatment:

- H1 - tempering at 950°C, cooling in water (fast)
- H2 - tempering at 950°C, cooling in oil (average)
- H3 - tempering at 950°C, cooling on the air (slow)

and some of them also:

- S1 - ageing at 500°C, cooling with the furnace
- S2 - ageing at 500°C, cooling on the air
- S3 - ageing at 700°C, cooling with the furnace
- S4 - ageing at 700°C, cooling on the air.

Changes in mechanical properties were the results of quenching. Properties obtained for each sample were taken into account:

- R_m [MPa] – strength
- $R_{0,2}$ [MPa] – conventional yield limit
- A [%] – extension
- Z [%] – contraction
- HB – hardness

Database created for the purpose of the experiments also includes the information on the chemical content of samples and their classification of the grade.

The present experiment is an example of a data source. In this case, the model is determined by the knowledge obtained from the research. The possibility of embedding it in terms of domain knowledge is provided by ontological model discussed before. An ontology written in OWL will allow to future integration of model of data structure with decision-making rules obtained from the processes of data mining. Such rules for instance may be extracted with algorithm of Classification and Regression Trees (C&RT).

The purpose of preliminary tests was to find relations between different types of quenching, and particulary to determine which processes has the most important influence on the desirable mechanical properties.

The algorithm of Classification and Regression Trees (C&RT) was used to acquire this knowledge. The aim of the model is to set the value of individual classes of dependent variables (R_m, $R_{0,2}$, A) formed on the basis of the conduct of the variability of the predictor variables (rate of cooling after tempering, type of modifier, temperature of ageing, the ageing rate of cooling). This will allow to construct the rules of inference based on four explanatory variables.

Cooling rate at hardening or ageing temperature are continuous variable, but the specifics of the process and characteristics of the collected data indicates that the selection was punctual (e.g. 500°C, 700°C and cooling in air, water, etc.). Therefore we treated these values as categories in qualitative variables in regression trees modeling.

As a result of the application of the algorithm of regression trees we obtained 19 rules, including:

- If the sample has been subjected to tempering H3 and ageing at 500°C, then the strength will have an expected value $E(X)$ = 476 MPa and variance $D^2(X)$=793
- If the sample has been subjected to hardening H3 and ageing in 700°C or without ageing at all, you will have the strength distribution of the average $E(X)$ = 530 MPa and variance $D^2(X)$=33
- If the sample modified with boron (K) was subjected to hardening H2, then the strength will have an expected value $E(X)$ = 577 MPa and variance $D^2(X)$ = 43
- If the sample modified with boron (K) was subjected to hardening H1, then you will have the strength distribution of the average $E(X)$ = 546 MPa and variance $D^2(X)$ = 2187
- If the sample not modified with boron (K) was subjected to hardening (H2 or H1), then you will have the strength distribution of the average $E(X)$ = 600 MPa and variance $D^2(X)$ = 325

The applicability of this knowledge in the system is provided, as it was mentioned, by the correct semantic description of the data structures. For this aim a transformation of the database schema to form of an ontology stored in OWL was made.

3.2. Transformation of relational database to the form of ontology

Schema of database created for the purpose of the experiments is shown in the Fig. 8.

Currently there are already known methods for semi-automatic transformation of database schemas into ontologies stored in the OWL language [5, 6, 7, 8]. Most of them, however, requires interaction with the ontology designer on one of the stages of transformation. It turns out that for simple databases, such a transformation can be successfully carried out manually, using tools for ontologies creation, and using the basic rules of transformation.

The first step is to save all the tables and individual fields in a graphic form. Most tables will reflect the future class. Liaison tables, which are the implementation of a many-to-many (n:m) relation form the basis for future relations in the ontology (*object properties*). A foreign key fields (foreign keys) will also establish a relationship in the ontology. This way the number of attributes in the schema obtaining the basis for future ontology can be reduced (Figure 9).

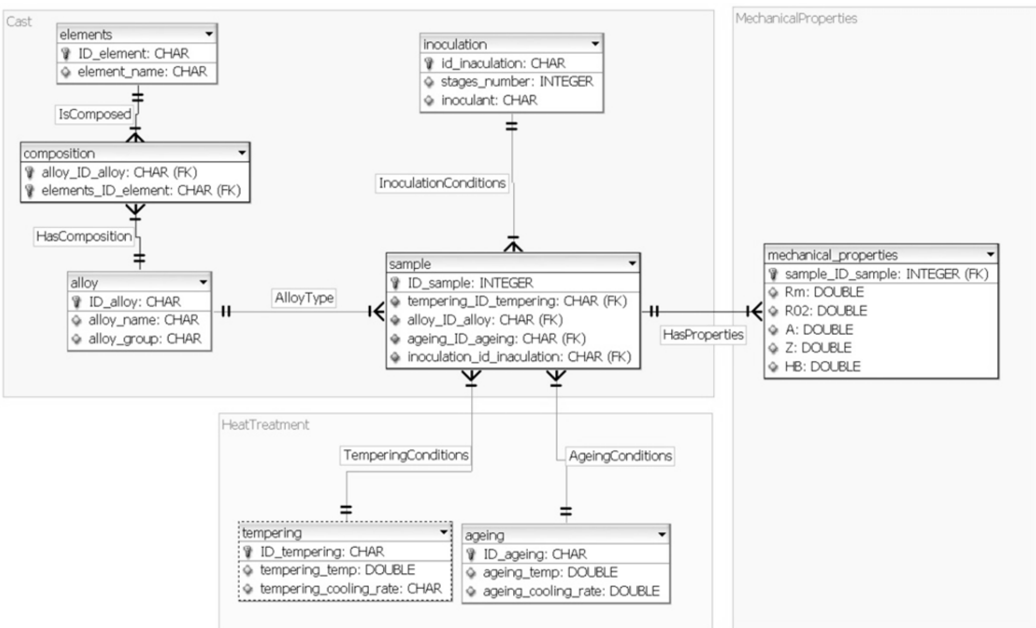

Fig. 8. Database schema for the experimental research on the mechanical properties of bronze BA1032

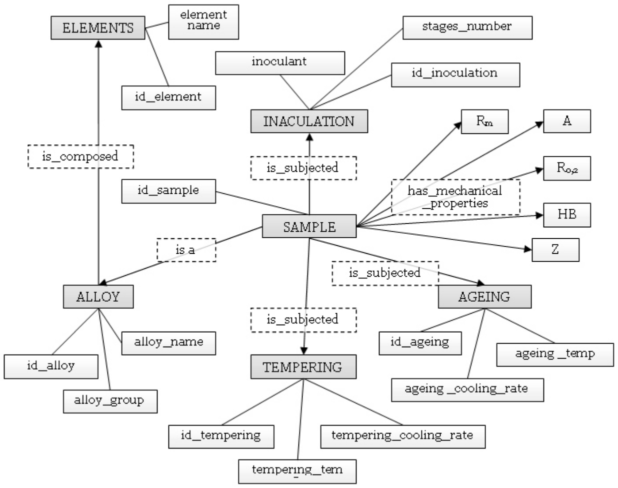

Fig. 9. First stage of transformation ER schema to OWL ontology

Tables, in which the foreign key is also the primary key, creates subclasses related in the ontology with *is_a* relationship. After transformations carried out in such way, we have to decide how to process the remaining fields. Some of them will automatically create the OWL *datatype properties*, but the designer may decide that the individual attribute is to become subclasses if it is relevant to the description field (Figure 10).

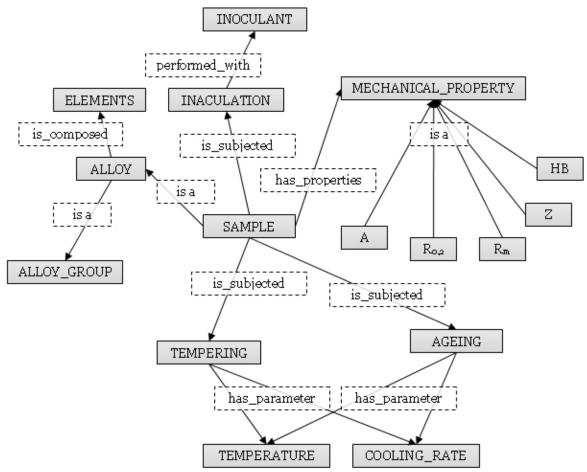

Fig. 10. Ontology graph retrieved from database schema

3.3. Editing an ontology

Thus prepared ontology schema can be edited in any OWL editor. In our case the Protégé 3.4 editor was used [4].

Correct description of each class includes the description of an object by *object properties* and *datatype properties*. The difference between these properties relies on the fact that the *object properties* associated with a given class use another class with relations.

Datatype properties allow to assign value the properties of a class that is given [11] (Figure 11).

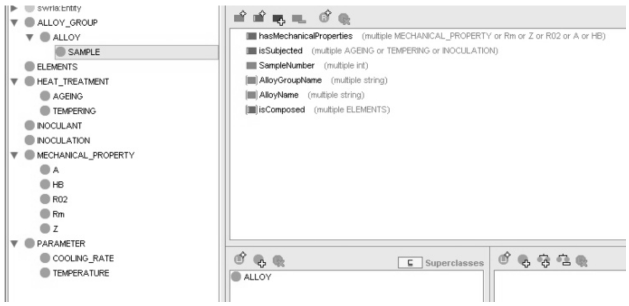

Fig. 11. Properties edited in Protégé 3.4

The next step is to map entities from the database for instances of classes in the ontology (Fig. 12). For this purpose you can use ready-made tools to speed up this process [7], or manually enter individual instances. Supplement instance is to adopt model for future treatment with the rules written in SWRL [8, 12], which is a further direction of research work.

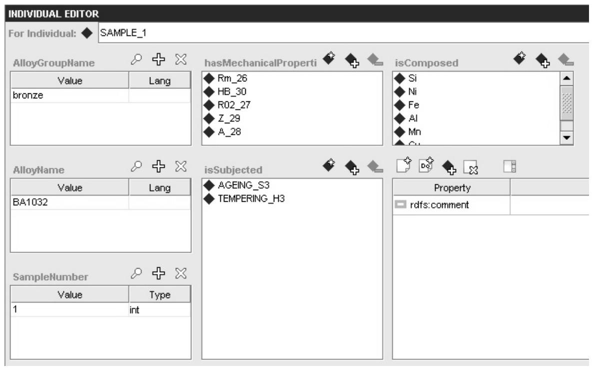

Fig. 12. Instances edited in Protégé 3.4

Excerpt from a sample description in OWL for the instance of element: Cu

<rdf:Description rdf:about="#Cu">
<isComponentOf rdf:resource="#SAMPLE_1"/>
<rdf:type rdf:resource="#ELEMENTS"/>
<hasName xml:lang="en">copper</hasName>
<hasName xml:lang="pl">miedź</hasName>
</rdf:Description>

4. The integration of domain knowledge and experimental data

In the issue of ontologies integration several approaches are established, e.g.:

- referencing upper ontologies
- importing completely upper ontologies into developed one
- creating a mapping ontology by binding an upper ontology with the domain ontology [13].

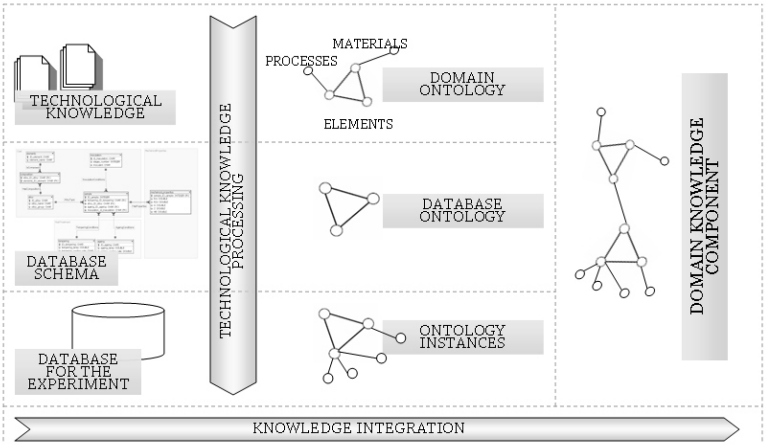

Fig. 13. The integration of domain knowledge and experimental data

In our case the most convenient way of integrating the domain ontology with the database ontology is to expand the former domain ontology with classes and properties from database ontology (Fig. 13). That approach leads to situation when our domain ontology is successively getting more specific instead of creating a single system ontology for every new experiment. Also the knowledge obtained from research works can be implant into the base ontology.

5. Conclusions

Meta-modeling used for domain ontology provides semantic description of the data obtained from material research works. Currently, ontologies are already the standard in creating a knowledge-based systems. They are the basic knowledge representation formalism which is able to provide so important and frequently requested knowledge reuse, sharing resources by different services and systems and system processing. One of accepted standard in this case is the OWL language, and its popularity testifies to the general need to develop shared standards of formalization of knowledge.

Further directions for research on ontologies in the areas of processing of copper alloys are inference models requesting the use of ontologies and SWRL rules.

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