NON-STRUCTURED MATERIALS SCIENCE DATA SHARING BASED ON SEMANTIC ANNOTATION

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ABSTRACT

The explosion of non-structured materials science data makes it urgent for materials researchers to resolve the problem of how to effectively share this information. Materials science image data is an important class of non-structured data. This paper proposes a semantic annotation method to resolve the problem of materials science image data sharing. This method is implemented by a four-layer architecture, which includes ontology building, semantic annotation, reasoning service, and application. We take metallographic image data as an example and build a metallographic image OWL-ontology. Users can accomplish semantic annotation of metallographic image according to the ontology. Reasoning service is provided in a data sharing application to demonstrate the effective sharing of materials science image data through adding semantic annotation.

Keywords: Non-structured data, Materials science image, Data sharing, Domain knowledge ontology, Semantic annotation, Metallographic image ontology

1 INTRODUCTION

Materials science data has been a valuable resource and the basis of modern material design, manufacture, development, and application (Westbrook, 2003). Their sharing has always been a focus of international research (Wei, Peng, Liu, & Xie, 2006), and the ways of sharing are mainly based on materials science databases (Ed, 2003). Non-structured data as an important category of scientific data is widely used in materials science; examples include phase diagrams, metallographic images, and CCT diagrams. Materials science image data are the basic data for analyzing material performance. While the development of computer technology enables the storage and distribution of materials science image data on an unprecedented scale, finding suitable materials science image data for a particular purpose is increasingly problem for materials researchers.

A major recent trend in the sharing of image data is to annotate those image objects. Image annotation is a process that supplements image data with literal description. Different types of descriptive information can be associated with images (Del Bimbo, 1999; Zachman, 1999), such as content-independent information, content-dependent information, and content-descriptive information. Content-descriptive information refers to content semantics and is concerned with relationships of image entities with real-world entities or temporal events, emotions, and meaning associated with visual signs and scenes (Liu, Zhang, Lu, & Ma, 2007). Content-descriptive metadata are the focus of this paper, and they can be specified using the following approaches.

In past studies, there are mainly three approaches for image annotation: keywords, free-text, and ontology. Image annotation based on keywords is an approach using keywords for image description, chosen arbitrarily from the vocabularies defined in advance. This has been done in the image retrieval domain by Gevers et al. (Gevers & Smeulders, 2000) and in the image motion estimation domain by Suzhou et al. (Zhu & Ma, 2000). If one is searching within a single image database that has been annotated carefully using a keyword vocabulary, then searching is simplified. Unfortunately, naive users do not necessarily know the vocabulary used to annotate an image collection, and this lack of keyword knowledge makes searching by text input more difficult (Hanbury, 2008). The IAPR-TC12 dataset of 20000 vacation images (Grubinger, Clough, Müller, & Deselaers, 2006) is described by free text, and each image is annotated in English, German, and Spanish. For this type of annotation, no pre-defined structure for the annotation is given. Thus users can annotate images using any combination of words or sentences. This method makes it easy to annotate images, but it is more difficult to use the annotation later in image retrieval because the free-text annotation is lacking in structure, concepts, and relationships.

An ontology is a specification of a conceptualization, where all the definitions are presented with respect to each other and their semantic relationships are defined explicitly (Jewell, Lawrence, & Tuffield, 2005). For that reason, ontology annotation is better than keywords annotation on knowledge representation of images. There exist a large number of studies on ontology-based image annotation completed in the last few years. Schreiber et al. (Schreiber, Dubbeldam, Wielemaker, & Wielinga, 2001) constructed a photo annotation ontology and subject matter ontology to help the annotation and retrieval of ape photos. Hollink et al. (Hollink, Schreiber, Wielemaker, & Wielinga, 2003) used SWI-Prolog to develop an RDF Parser, which was used to accomplish the annotation and retrieval of artistic images. In the CONFOTO project (Nowack, 2006), an OWL ontology, annotation parser, and RDF metadata were all converted into components, and these components were used successfully in the annotation and sharing of conference-related photo and video over the web. Khan et al. (Khan, 2007) registered knowledge ontology as a web service to an intelligent agent center, with an agent responsible for annotating athletic images on the web.

Semantic web technology makes creating a syntactic format specifying background knowledge for image data possible, and many research effects have shown that an ontology is a proper basis for semantic annotation of images. The annotation of materials science images involves paying attention to domain knowledge representation, which is different from general annotation. The implicit knowledge of materials science imaging should be expressed explicitly in the annotation. Therefore semantic annotation based on an ontology is the most suitable approach. Research on the semantic annotation of materials science image data has been rare, however, and furthermore there is no mature domain knowledge ontology at present for this annotation.

In this article, we explore the approach of knowledge presentation for materials science image data, and propose a semantic annotation method for materials science image data based on an OWL ontology. Then, reuse of the knowledge of a materials science image is resolved by DL reasoning in TBox (Horrocks, 2002). Finally, using metallographic image data as an example, we build a metallographic image ontology and develop an annotation and query tool to help users annotate and share the metallographic image data. The following sections of this paper describe an overview of the approach used in our study, the ontology-based annotation mechanisms, and a semantic query example.

2 OUR APPROACH

Current materials science image data services systems focus strongly on databases for specific materials, which can not meet the requirements for materials researchers. Materials scientists do not have timely access to the experimental results generated by different research institutions. Convenient retrieval of high-quality materials science image data directly impacts the sharing of materials science image data. The following scenario is common in materials science research. A user obtains a microstructure image of 20 steel by metallographic testing and wants to compare it with previous results, in order to estimate the heat treatment technique used in the metallographic test. We can construct a query: *Which type of heat treatment is shown in the 20 steel metallographic image? This image* *shows a homogeneous distribution of ferrite (white) and pearlite (black).*

The user can obtain knowledge about the above metallographic image by searching for an image with the same content. The result shows that a homogeneous distribution of ferrite (white) and pearlite (black) of 20 steel is obtained by normalizing at 890°C for 30 minutes and air cooling. Users are concerned more with obtaining the materials science image in this scene; therefore, the annotation of the matching materials science image should be able to express additional implicit knowledge. To simulate this process and create our test case, we obtained about 1000 images from a metallographic image database and used a subset of approximately 100 metallographic images of common steel for annotation.

The main targets of our annotation study include: 1) building a knowledge ontology to express implicit knowledge of metallographic images, which can meet the requirements of the user demand for materials domain knowledge; 2) deducing relevant knowledge of metallographic images from the semantic annotation information, which can enrich the semantics of materials image data and realize the full value of the data by increasing the usage of generated data; 3) implementing a semantic annotation architecture, which can integrate the distributed materials science image data into a whole. Figure 1 shows the annotation architecture used for data sharing. The ontology-based semantic annotation system has a four-layered architecture, including an ontology building layer, semantic annotation layer, reasoning service layer, and application layer.

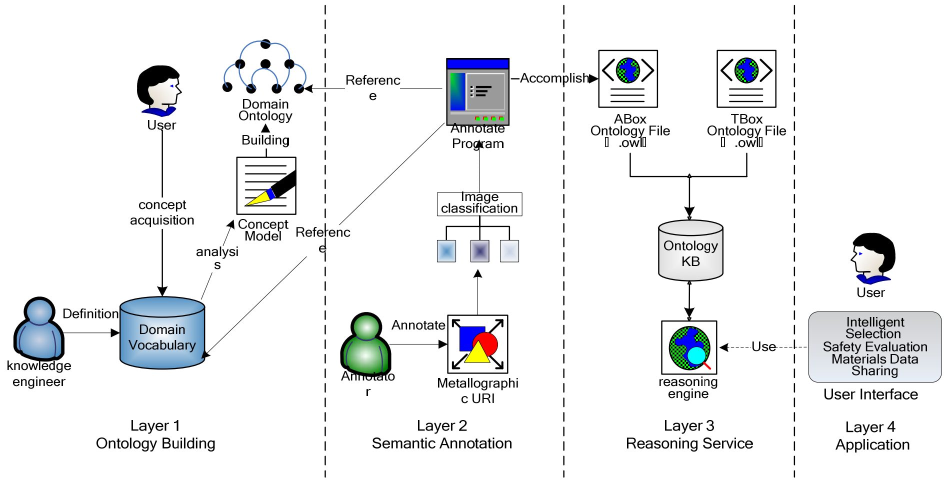

Figure 1. Ontology-based Semantic Annotation System Architecture

The ontology building layer uses a user-cognition-based approach for knowledge presentation of various non-structured data. The prerequisite for building a knowledge ontology is the extraction of concepts. Most research has so far used expert knowledge to give direct definitions to knowledge ontology. This creates difficulty for users in finding the images they need due to the differences between user cognition and that of domain experts. Thus we attempt to build the metallographic image knowledge ontology based on user-cognition.

The image metadata is archived into an ABox (Horrocks, 2002) file of OWL ontology through annotation program in the semantic annotation layer. In this layer, the annotation template is designed according to the concepts of metallographic image; metallographic images are annotated, and we represent them in ontology languages such as OWL for machines to read, so as to raise the annotated image data from descriptive to knowledge expression.

In the reasoning tier, all image data have a set of semantic annotation metadata stored in an OWL format that form a knowledge base using TBox. Reasoning service is provided to define rules to carry out queries and knowledge reasoning related to metallographic image. In this layer, the knowledge base provides a test service that can be used to test instances as fitting to certain concepts or relationships when reasoning. The results of reasoning (i.e., knowledge about a metallographic image) can be reused in the application layer. A powerful client is provided for users to query and acquire their desired metallographic image data for applications such as intelligent selection, safety evaluation, and materials science data sharing.

3 ONTOLOGY-BASED METALLOGRAPHIC IMAGE ANNOTATION

Generally, annotation is a process to describe image content; however, for science data, it is a knowledge representation process. The ontology-based metallographic image annotation has three steps: 1) analysis and definition of the conceptual structure (i.e., knowledge ontology); 2) provision of a template for metallographic image annotation according to the defined ontology; 3) understanding and reasoning about metallographic image knowledge, achievable when we use logical calculation in specific applications.

3.1 Metallographic Image Ontology Building

Ontology-based annotation is relatively new, and there are no existing ontologies for metallographic images. Thus we decided to define the metallographic image ontology on the basis of a cognitive analysis of user perspective. In this section, we describe building a metallographic image ontology. Definitions of this ontology are as follows according to the domain concepts collected and screened by knowledge engineers:

Definition 1. Suppose O is a metallographic image ontology, which is defined as a 4-tuple O=<C, H^c, DP, OP>, where C is a finite set of concepts of metallography domain, for example, grain size, network carbide, on-metallic inclusion, depth of decarburized layer; H^c is the hierarchical relations of concepts sets; DP is a finite set of relations among concepts and data types; and OP is a finite set of relations among objects.

Definition 2. The concept of an ontology is defined as a triple C_i=<$CNAME_i$, CID_i, A_i>. $CNAME_i$ is the name of concept i; CID_i uniquely represents a concept of metallographic ontology; and A_i is a logic axiom set of C_i.

Definition 3. The hierarchical relation of concept C is defined as H^c. For example, H^c (C_i, C_j) shows that C_i is the father concept of C_j. Figure 2 shows the taxonomy of metallographic image concept.

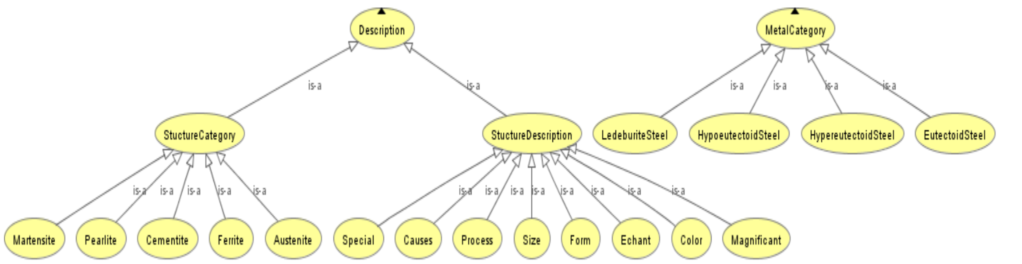

Figure 2. The hierarchical relation of concepts of metallographic image

Although there is a conceptual category, the simple hierarchical relation can not express the semantic relations. Therefore, we define sets of DP and OP to perfect the semantic relations among concepts.

Definition 4. DP is a finite set of relations between concepts and data types. For example, ***hasURI*** is the relation between the instance of class ***metalcategory*** and the datatype ***xsd:AnyURI***; ***hasName*** is the relation between the instance of class ***metalcategory*** and the datatype ***xsd:String***; ***hasURI*** and ***hasName*** are defined as functional properties, so for a given individual, there can be at most one individual that is related to the individual via these properties.

Definition 5. OP denotes non-hierarchical relation among objects. For example, the property ***hasClass*** and ***isClassOf*** denote a subordination relation between class ***metalcategory*** and class ***structurecategory***. ***hasClass*** and

isClassOf are defined as inverse properties, that is to say, the property ***hasClass*** is an inverse property of the property ***isClassOf*** . If *T10 image* **hasClass** *Pearlite*, then because of the inverse property we can infer that *Pearlite* ***isClassOf*** *T10 image*.

We specified our metallographic image ontology in OWL using Protege3.1 according to the above definitions. That is to say, we defined the TBox of our metallographic image ontology, including all classes of metallographic image ontology and corresponding datatype property, object property, and asserted conditions. Figure 3 shows the class and property hierarchy of metallographic image ontology.

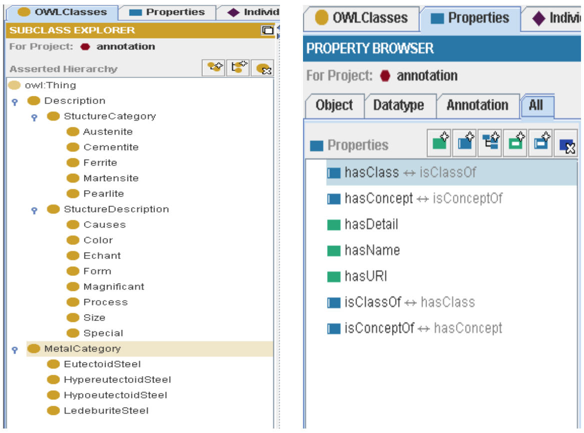

Figure 3. The class and property hierarchy of metallographic image ontology

3.2 Annotation Template of Metallographic Image

Annotation of metallographic image is a process, in essence, to add semantics to metallographic images. For this purpose, we developed an annotation tool that provides the annotator with a description template derived from the defined metallographic image ontology. Figure 4 shows the semantic annotation framework based on ontology.

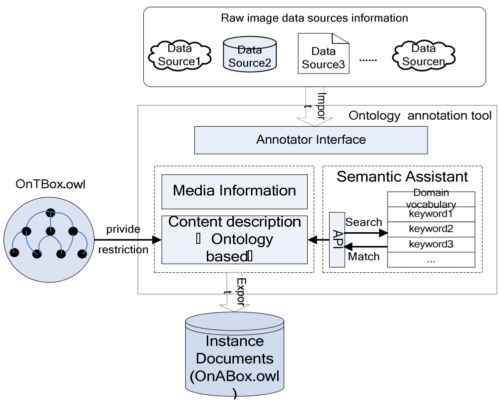

Figure 4. The semantic annotation framework based on ontology

The tool we developed reads a TBox file containing OWL ontology specifications. From the OWL specifications, the tool generates a user interface for annotating images. In view of different levels of knowledge possessed by different annotators, a semantic assistant was developed to improve the precision of annotation. The assistant provides a domain vocabulary as a reference service for annotators, and the vocabulary can be considered as an instance vocabulary of the domain ontology. Each annotated item is in correspondence with several example instances in domain vocabulary, e.g., the item 'carbon structure steel grad' is bound with specific grades in the domain vocabulary, such as Q195, Q215, Q235, Q255, and Q275. Users can type in a term and use the domain vocabulary to raise both annotation and recall precision. The storage of annotated information is an important part of the framework, and it is done in either internal or external ways. Although the internal way is easy to realize, the convenience is offset by the burden of extra data processing to update annotated information in original metallographic images once a targeted domain changes the requirements. Thus we use external storage to separate annotated information and original metallographic image data, catering to the variability of metallographic practices.

Semantic annotation in our design is a process of creating ontology instances. Thus the semantic metadata items to be annotated need to be in one-to-one correspondence with concepts in the metallographic image ontology. Every annotated metallographic document is an individual file of the metallographic image ontology, which is divided into two parts: ABox and TBox. The predefined image ontology is TBox; the annotated information is ABox, and they are explicit representations of knowledge of metallographic images. Meanwhile, in the reasoning tier, implicit knowledge of metallographic images can be found by a reasoner based on the ABox and TBox. Figure 5 shows the annotation tool prototype, which is an interactive and Java-based annotation form. The figure also illustrates how several techniques are combined to improve the user's experience, such as reading the ontology, importing raw image data, writing an instance of ontology, and checking the consistency of an instance file.

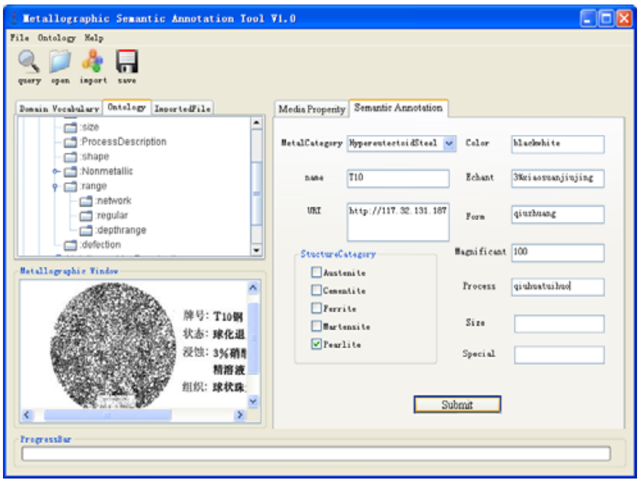

Figure 5. The annotation tool prototype. The user has selected T10 steel metallographic image as the object, and the semantic annotation according to the metallographic image ontology has been done.

3.3 Reasoning Rule Design

If the reasoning engine can be seen as a semantic bridge between the annotated information and its application, then the reasoning rules are the supporting piers of the bridge. The reasoning engine conducts semantic reasoning with the metallographic knowledge base by defining a series of reasoning rules based on the content of the ABox and TBox of the ontology. The purpose in designing reasoning rules is to obtain more relevant research results to meet users' requirement for knowledge about metallographic images.

Semantic reasoning occurs when users submit a query or when semantic annotation is finished. At this phase of user interaction, a user query is decomposed and extended into many sub-queries, and then returned results are obtained by semantic reasoning. This method greatly enhances the recall precision rate, but system performance may be subject to obvious degradation when there are many concurrent users. Another method of semantic reasoning can be performed as soon as the annotation is finished. The relationship among concepts can be handled, but the relationships among individuals can not. Considering this, semantic reasoning is divided into two phases: TBox reasoning and ABox reasoning. TBox reasoning is responsible for handling synonymous and generalization relationships among concepts when annotation is accomplished. ABox reasoning is responsible for handling queries based on an ontology instance. In addition, because special concepts in metallography are not changed easily, the results of TBox reasoning are rarely changed. All kinds of metallographic images emerge, however, continuously with the development of new materials. Thus the results of ABox reasoning usually change over time correspondingly. We differentiate between ABox reasoning and TBox reasoning, which can reduce repetitive work and improve the efficiency of semantic reasoning.

The design of reasoning rules has been decomposed into TBox reasoning rules and ABox reasoning rules, respectively. The former are defined in advance in a rule database, and the latter are user-defined rules aimed at a specific application. Jena (McBride, 2004), developed in the HP laboratory, can provide support for TBox reasoning, and one of the services offered by the reasoner is to test whether one class is a subclass of another class. By performing such tests on the TBox of ontology, it is possible for a reasoner to compute the inferred ontology class hierarchy. The task of computing the inferred class hierarchy is also known as classifying the ontology. Furthermore, the classification information can be reused without reasoning at the phase of user query.

Ontology information includes abundant knowledge that is not directly expressed. But knowledge discovery is a high-cost activity due to its very complex reasoning process. If knowledge discovery is supposed to happen during retrieval, the efficiency of the retrieval will be low. Our way of dealing with this is to first discover the knowledge in ontology by using Jena. Although the flexible application of the rules defined above in Jena can satisfy most reasoning needs, their use is limited in certain types of applications. Therefore, users are able to achieve better adaptability and extensibility through self-defining reasoning rules (i.e., ABox reasoning rules). According to the specific needs, three extensive rules of semantic reasoning are created as follows:

Rule 1: (? *x* ***viaHeattreatment*** ? *y*), (? *y* ***subclassof*** ? *z*)—> (? *x* ***viaHeattreatment*** ? *z*)

Rule 1 is a semantic entailment rule. Suppose that *y* is the heat treatment process of metallographic image *x*. While *y* belongs to *z*, then *z* is also the heat treatment process of *x*. For example, if you search T10 steel with annealing metallographic image, you could find metallographic images with other heat treatments, such as normalizing and quenching. Annealing, normalizing, and quenching all belong to the overall heat treatment.

Rule 2: (? *x* ***refersTo*** ? *y*), (? *y* ***sameAs*** ? *z*)—> (? *x* ***refersTo*** ? *z*)

Rule 2 is a synonym expansion rule. Suppose that *y* is the microstructure of metallographic image *x*. While *y* is equivalent to *z*, then *x* contains *z*. For example, an image shows microstructure *P*, and *P* is the abbreviation of pearlite; then the image showing pearlite can be found.

Rule 3: (? *x* ***onlyBelongto*** ? *y*), (? *y* ***storedplaceIs*** ? *z*) —> (? *x* ***storedplaceIs*** ? *z*)

Rule 3 is a semantic association rule. Suppose that *x* is a metallographic test result, and *x* only belongs to a certain type of metallographic image *y*. While *y* is stored in *z*, then *x* is also stored in *z*. For example, macrostructure defect images are stored in the macrostructure defect images database. A macrostructure defect image of T10 steel belongs to macrostructure defect images; then it is stored in macrostructure defect image database.

4 QUERY BASED ON SEMANTIC ANNOTATION

The semantic annotation of metallographic images based on an ontology is essentially a process of knowledge representation and reuse. Image description equipped with a formal logic-based semantics is one of the key features of semantic annotation. Another important feature is that the semantic annotation information can be seen as a knowledge base, and implicit knowledge about a metallographic image can be inferred from the knowledge base. Meanwhile, self-defined semantic reasoning rules can meet the requirements of many expansion queries, such as semantic implications, semantic extensions, and semantic relativity. Consequently, metallographic image data can be retrieved more effectively using the semantic annotation and reasoning mechanism.

We have developed a semantic retrieval system with metallographic image data as an example, to validate whether the annotation method is feasible for sharing non-structured materials science data. The user interface is built with Java SWT, and we use pellet (Sirin, Parsia, Grau, Kalyanpur, & Katz, 2007) as the OWL reasoner and Jena ARQ as OWL API for the query engine. In order to demonstrate the advantages of semantic annotation for metallographic image retrieval, we construct queries based on user-habit. Assuming a user wants to find a metallographic image which belongs to hypoeutectoidsteel, the user would enter a keyword such as *HypoeutectoidSteel*. The answer wanted, however, is some specific instance of *HypoeutectoidSteel* and some relevant knowledge of the instance. Figure 6 shows the results of semantic association query.

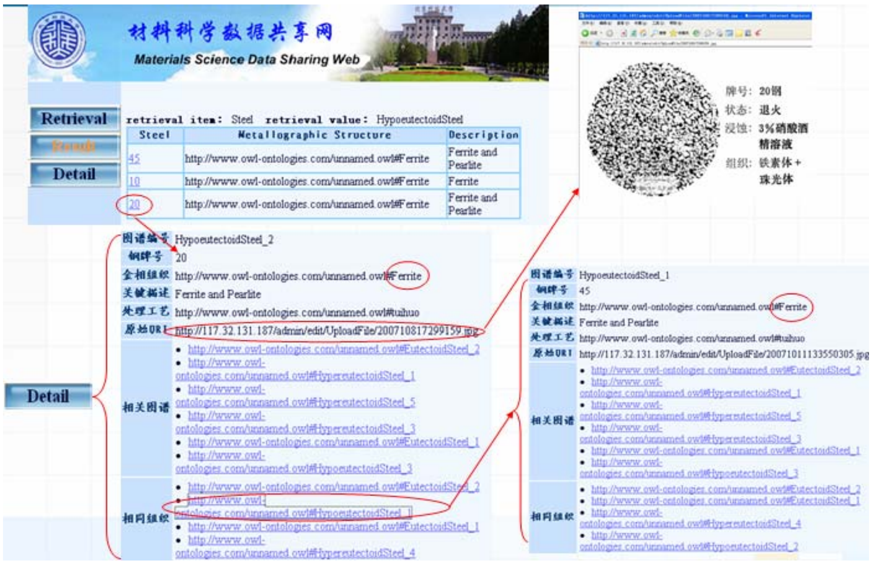

Figure 6. The results of semantic association query. In this process, we can derive a semantic match with the concept *HypoeutectoidSteel*, and we can find more relevant information by semantic association retrieval.

The above query result is derived from the rules we have defined. By inference engine, the result of query *HypoeutectoidSteel* is as follows: *45 steel*, *10 steel*, and *20 steel*. They are all instances of the concept *HypoeutectoidSteel*. Furthermore, more relevant information about this instance image can be obtained. For instance, *45 steel* can be found in the detail information for *20 steel* by semantic association retrieval because *45 steel* and *20 steel* have the same microstructure, ferrite and pearlite. In contrast, the general image search engine is only to find the items including keyword *HypoeutectoidSteel*. Although the SPARQL statement of the semantic query is similar with the SQL query, in fact the SPARQL query in the web has greater flexibility. Because all kinds of web data are combinations of external data sources, they can not be predicted nor are they reliable. As far as a query is concerned, SQL is not suitable for dynamic querying of the web data because its pre-defined structure, which satisfies constraint completeness, is fixed. In addition, the processing objective of SPARQL and SQL is different. Further relationships are not derived from the simple association rules of SQL, but SPARQL is provided with reasoning abilities by virtue of rules definition. Consequently a semantic query based on SPARQL can improve precision rate, and the semantic query process based on user cognition can provide users with additional interesting answers, which would not be requested in inquiry by reasoning rules.

5 CONCLUSION AND FUTURE WORK

In this paper, we have presented an ontology-based approach that can be used to develop annotation for non-structured materials science data with the usage of semantic web technologies. The role of ontology-based techniques is to exploit a specialization representation of materials science image content, and to form a knowledge base of non-structured materials data. The semantic web technology is increasingly important for annotation of non-structured data into machine-readable formats. Furthermore, semantic annotation allows us to make use of concept searches instead of keyword searches. Also, it paves the way for more specific applications. Taking metallographic image data as an example, we have implemented a semantic annotation tool based on a metallographic image ontology and developed a semantic query prototype system to evaluate the efficiency and effectiveness of our method. The results showed that image query based on semantic annotation has a high precision rate.

Future enhancements will focus on three issues. The first major target is to acquire more accurate domain knowledge representation by using formal concept analysis. The second is to propose an application standard similar to DICOM (Digital Imaging and Communications in Medicine) to assist annotation of materials science image data. The third is to explore an automatic annotation approach that is able to intelligently annotate non-structured data using manual training in conjunction with feedback.

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