

STSM: An Infrastructure for Unifying Steel Knowledge and Discovering New Knowledge

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Abstract

There are rich data resources in materials science, but these data resources are heterogeneous in level of system, structure, syntax, and semantics. Therefore, a domain ontology is necessary and helpful for the integration of these heterogeneous data resources, and it is also one of the main tasks of materials informatics. In this paper, we propose a steel semantic model (named STSM) based on ontology and logic rules for the representation of the steel knowledge. STSM is developed with the consideration of the features of materials data and the developed process is presented. Then, we describe the content and organization of STSM which covers the basic knowledge in steel domain. Further, domain axioms and logic rules are designed to enhance the reasoning ability of STSM. STSM is built and tested in protégé, and an experimental prototype based on Jena is also developed to demonstrate the effectiveness of STSM.

Keywords: *domain ontology; steel knowledge; domain axioms; rules; reasoning*

1. Introduction

Materials data resources are playing an important role in science development and there are more and more materials information available on the web. However, these resources have different kinds of formats, and they are lack of unified standard [1], which may lead to difficulties in finding materials information. Most of the time, materials researchers have to go to different web sites or knowledge bases to query knowledge of interest, which is inconvenient. Moreover, the existing materials query patterns which can support reasoning are very few. Reasoning is very important for materials researchers, because it can reveal the implicit materials information to researchers by imitating human intelligence [2]. Therefore a materials domain ontology which can support reasoning should be constructed to integrate heterogeneous materials data resources and find new knowledge or implicit knowledge from existing knowledge bases [3-6]. This paper chooses steel domain as the research object, and the steel semantic model is constructed to integrate steel knowledge. Moreover, the steel semantic model includes domain axioms, and the rules are also designed. This paper makes the following contributions.

(1) We describe the development process of steel domain ontology based on the Methontology method [7] which provides guidelines for constructing domain ontologies.

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(2) We develop the steel semantic model STSM. STSM covers comprehensive and shared knowledge in steel materials domain, so it can be used to integrate heterogeneous materials data resources in semantic level.

(3) The axioms and rules are designed in STSM, and they can be used to reclassify and find new knowledge from existing knowledge bases. Furthermore, we discuss the application of axioms and rules in steel domain.

The remainder of paper is organized as follows. Section 2 introduces the related work. Section 3 describes the problem definition and important concept definitions. Section 4 gives development steps, content and organization of STSM. Section 5 shows the design and application of axioms and rules in steel domain. Section 6 concludes the paper and gives future work.

2. Related Work

In recent years, relatively mature domain ontologies have been established in environment [8], biology and medicine [9-22], chemistry [23-26], art [27] and other domains [28] with the rapid development of semantic web technology, and they have been applied to their respective domain. However, materials domain may have few relatively mature ontologies [29-31]. In materials domain ontologies, Ashino establishes a more comprehensive materials ontology [1], and it can cover completely materials knowledge and be used for exchanging data. MatONTO [32] is mainly used to study information integration about inorganic materials, which can support rules and be used to discover new compounds. MatOWL [33] explores the transformation from MatML to MatOWL and the population of instance data from MatML to MatOWL. The Steel ontology in ONTORULE [2, 30, 34, 35] includes less concepts, which focuses on the reasoning applied in engineering. These materials domain ontologies promote the development of materials data integration, but some of them lack of domain axioms and rules or have fewer concepts. Moreover, the reasoning ability is limited. Therefore we try to construct a steel semantic model which includes more comprehensive domain concepts and supports axioms and rules, so that materials researchers can discover new materials knowledge by axiom-based or rule-based reasoning.

3. Problem Description and Concept Definition

3.1. Problem Description

Immeasurable amounts of steel materials data are accumulated by different kinds of institutions, and lots of them are open. However, these open data resources are heterogeneous in level of system, structure, syntax, semantic. Most of existing materials domain ontologies are not specially designed for steel knowledge, so they may not summarize the comprehensive steel knowledge. In addition, some of existing materials ontologies may not support axioms or rule-based inferences. Therefore it is necessary to create a steel semantic model for integrating the heterogeneous data resources and finding new knowledge from existing knowledge bases. The following goals are expected to be achieved in this paper.

(1) A relatively comprehensive steel semantic model (we will extend to the field of metallic materials domain in the future) should be established, and it can cover the basic concepts of steel domain and the relationships between these concepts.

(2) The steel semantic model should include axioms. We can achieve reclassification by axioms. For example, the concepts which meet the axiom about dual-phase steel will be reclassified as subclasses of dual-phase steel.

(3) The rules are also designed in steel semantic model. Some inferences are too cumbersome to be represented by axioms, and it is necessary to use rule-based reasoning. We can find hidden materials knowledge by logic rules.

(4) The steel semantic model is constructed with comprehensive concepts and relationships from existing steel knowledge. We also refer to other related materials semantic model, so it can be compatible with other major materials ontologies, which makes it easy to map with other materials ontologies.

3.2. Conception Definition

It is necessary to explain the following definition for convenient expression in the next subsections.

Definition 1. Ontology. Ontology includes a series of finite terminologies and relationship between terminologies [36,37,38]. Ontology O can be represented as a quintuple: $O = (C, I, P, A)$, where C represents the concept set. I represents individual set, and i represents instance($i \in I$). P represents property set, and $P = P_o \cup P_d \cup P_a$, where P_o represents object property set and it is used to represent relationship between two instances($i1, i2 \in I$); P_d represents data property set and it is used to represent relationship between instance and data value; P_a represents annotation property set. A means axioms set.

Definition 2. STO. Based on Definition 1, we give the definition of the steel ontology STO: $STO = (C_{st}, P_{st}, I_{st}, A_{st})$. C_{st} means concept set of steel domain, which covers the basic terminologies in steel domain; P_{st} represents property set of steel domain; I_{st} represents individual set of steel domain; A_{st} represents axioms set, and $A_{st} = A_r \cup A_d$, where A_r represents restrictive axioms set and A_d represents defined axioms set which consists of domain axioms.

It should be pointed out that the rules in steel semantic model are implemented by Jena Rule, so they are not parts of STO. Therefore steel semantic model STSM is defined as follows.

Definition 3. STSM. $STSM = STO \cup R_{st}$, where R_{st} means rules set. Further, $R_{st} = R_c \cup R_p$, where R_c represents classification rules set and R_p represents prediction rules set.

Some important concepts such as A_d and A_r in above definitions should be explained in more detail. The defined axioms A_d is presented in the form of necessary and sufficient condition, and it is an equivalent relation. The part of the left side of the equation is defined concept which is always the abbreviation of complicated description. Correspondingly, the part of the right side of the equation is made up of atomic terms or properties from O . The restrictive axioms [39] A_r is used to describe various restrictive condition of concepts, and it includes value restrictive and cardinality constraint [40]. The value restrictive is used to restrict domain and range of attribute, and cardinality constraint is used to limit the number of attribute value.

Further, classification rules R_c is used to reclassify according to different standards. For example, if a steel material's tensile strength is greater than 1400Mpa and G_r content is greater than 10.5%, then it is a *super high strength stainless steel*. The prediction rules R_p can predict unknown phenomenon or properties by relevant historical data and existing data.

4. Design of STSM

4.1. The Development Process of STSM

With the consideration of the feature of materials knowledge, we develop STSM based on the guidelines of methontology method [7,41]. According to the proposed methods, STSM has been developed. Table 1 gives the development steps of STSM, and Figure 1 describes the development process of STSM in the form of graph in detail.

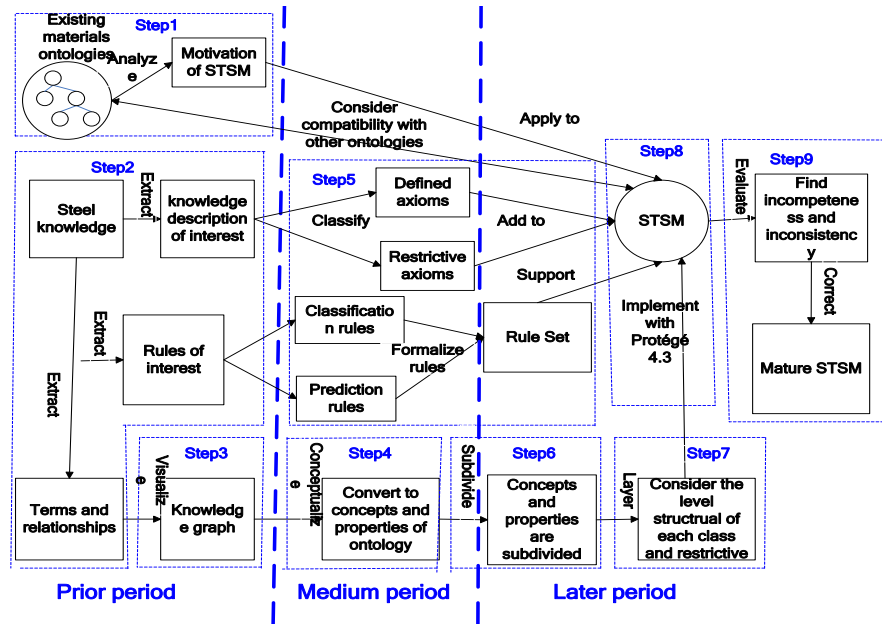


Figure 1. Development Process of STSM

Table 1. Development Step of STSM

Steps	Description
Step1	The existing materials ontologies are analyzed and the motivation of STSM is confirmed.
Step2	The steel materials knowledge is analyzed and terminologies and relationships are found.
Step3	The terminologies and relationships are represented in the form of graph
Step4	The terminologies and relationships from topological graph are converted into concepts and properties from STSM
Step5	Relevant axioms and rules are made.
Step6	STSM can be subdivided into several major classes, and we should consider relationships between different classes.
Step7	The hierarchies in each major class should be considered, and corresponding cardinality constrains and value limitations should be made.
Step8	Implementation stage. OWL ontology is generated with Protege4.3
Step9	Evaluation stage. The inconsistency and incompleteness are evaluated through the relevant technology with the participation of domain experts

In step 2, the knowledge topological graph of steel materials is generated as Figure 2 by analyzing steel materials knowledge. In Figure 2, the rounded rectangles represent materials

properties such as basic data, heat treatment, chemical composition, mechanical property, processing property etc. Rectangles represent specific properties in detail. Ellipses mean steel classification which includes structural steel, machine parts steel, tool and mould steel, heat resisting steel and stainless steel.

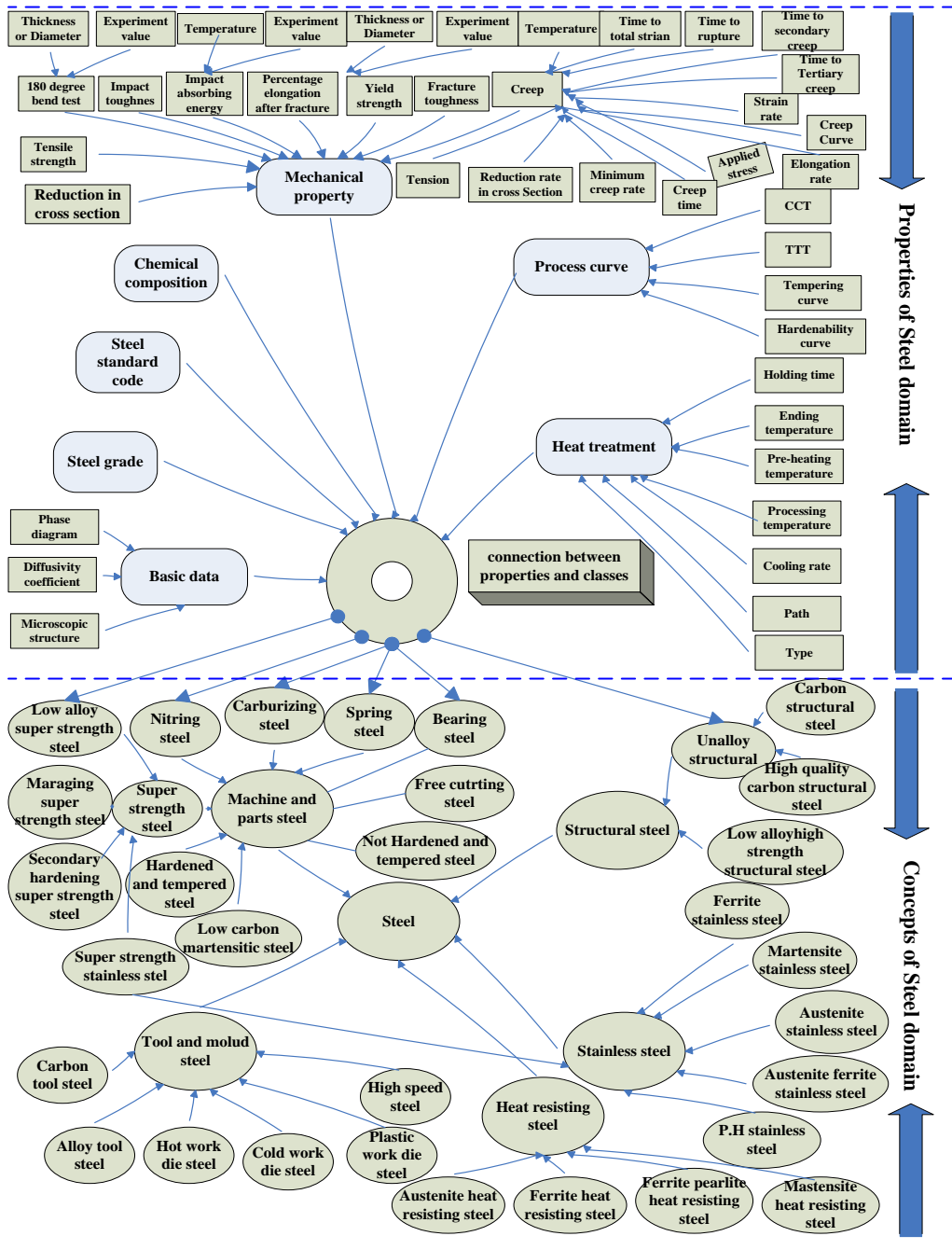


Figure 2. Knowledge Topological Graph of Steel Materials

4.2. Content and organization of STSM

Currently, STSM includes steel ontology STO and rules set R_{st} . Now STSM has 476 concepts, 46 object properties and 24 data properties, and it can cover the basic knowledge of steel materials. Figure 3 shows organization structure of STSM. Obviously, STO is the core in STSM and it supports rules. In detail, concept set C_{st} includes 4 basic classes, and they are *Element* (it includes basic chemical elements), *Property* (it includes basic materials properties), *Steel* (it is classified into different categories according to different standards) and *Unit*. Specially, *Property* and *Steel* are key classes in STSM and introduced in the following.

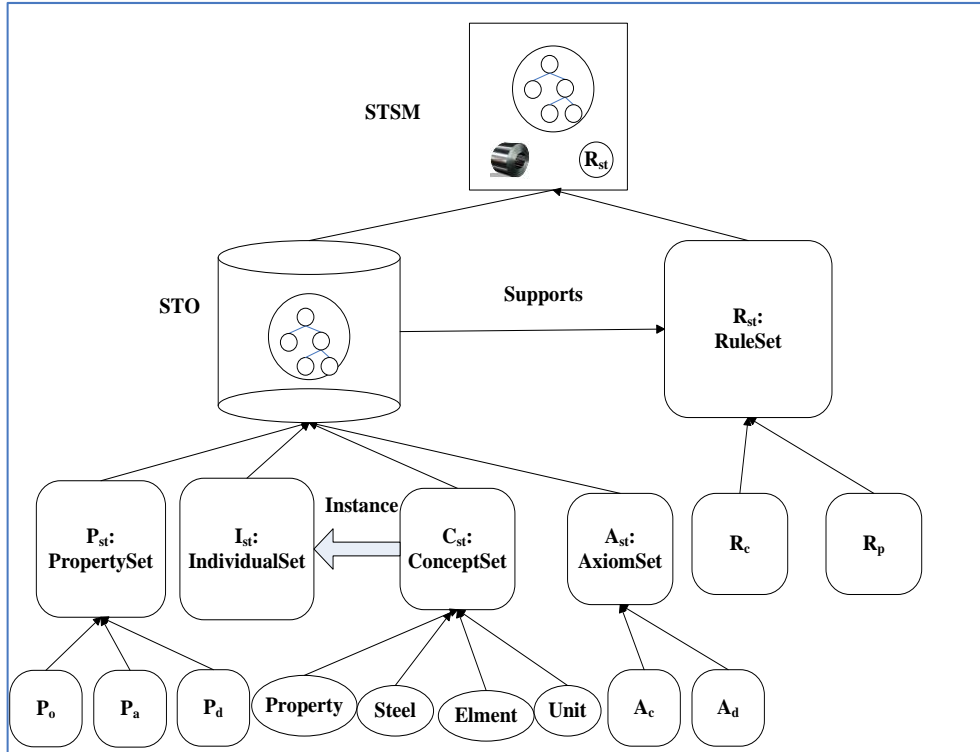


Figure 3. Organization Structure of STSM

Property class is mainly based on the properties of steel materials, and main properties in steel are represented in the form of ontology languages. With the help of the subclasses of *Property*, the properties of steel materials are represented clearly. Figure 4 gives the organization structure of *Property*. The subclasses of *Property* consist of basic data, chemical composition, mechanical property, process curve, heat treatment and physical quantity. Basic data includes microstructure, diffusivity coefficient and phase diagram, and they can also be subdivided. For example, microstructure can be subdivided into 2D micro structure and 3D micro structure. The mechanical property includes yield strength, fracture toughness, 180 degree bend test, tensile strength etc. The process curve includes TTT, CCT, tempering curve, harden ability curve. The physical quantity includes time, diameter, and temperature etc.

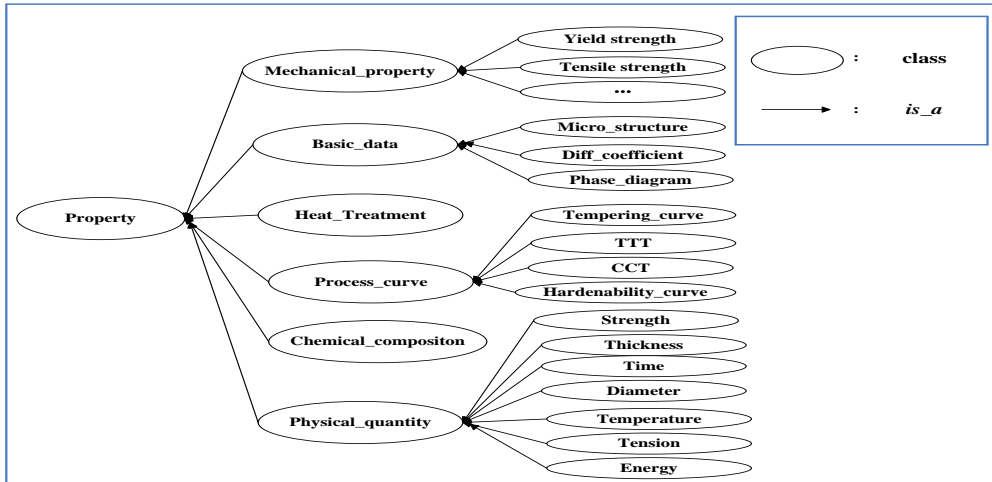


Figure 4. Organization Structure of Property

Furthermore, *Steel* is also the core class in the STSM. The steel domain has different classification methods according to different principles. For example, the *Steel* can be classified according to application, organization structure and different standards (For example, the steel serial number standard from America is used to classify in steel domain). So different classification principles should be considered in *Steel*, and the *Steel* is classified according to application of steel in this paper, and other classification methods are given in the form of axioms or rules. The Figure 5 shows organization structure of *Steel* according to application of steel. *Steel* has subclasses such as structure steel, machine parts steel, tool and mould steel, stainless steel and heat resisting steel. Structural steel can be also classified into unalloy structural steel and low alloy structural steel. Machine parts steel includes spring steel, bearing steel, carburizing steel, hardened and tempered steel and so on. Similarly, tool and mould steel, heat resisting steel and stainless steel have also different subclasses.

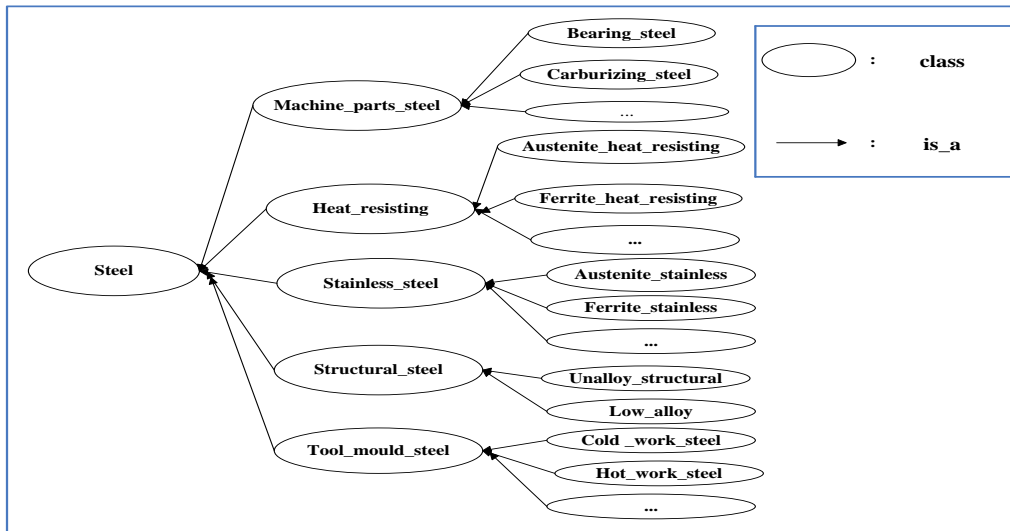


Figure 5. Organization Structure of Steel

Table 2 presents the important classes of STO along with their direct parent class, and through this table we can clearly see the hierarchical structure of the core concepts and relationships between them in steel materials. For example, the direct children of *mechanical property* include fracture toughness, impact toughness, creep etc, and it has also direct parent class *property*. Likewise, the direct parent class of high quality carbon structural steel and carbon structural steel is unalloy structural steel which has structural steel as its direct parent class. Table 2 may not show the relationships between these important concepts, so Figure 6 complements the relationships.

Table 2. The Classes and their Direct Parent Classes in Steel Domain (part)

The important classes of STO	Direct parent classes
diffusivity	Property
Microscopic_structural	Property
Heat_Treatment	Property
Mechanical_property	Property
180-degree_bend_test	Mechanical_property
Creep	Mechanical_property
Fracture_toughness	Mechanical_property
Impact_toughness	Mechanical_property
Tensile_strength	Mechanical_property
Yield_strength	Mechanical_property
Structural_steel	Steel
Low_alloy_high_strength_structural_steel	Structural_steel
Unalloy_structural_steel	Structural_steel
Carbon_structural_steel	Unalloy_structural_steel
High-quality_Carbon_structural_steel	Unalloy_structural_steel
Machine_parts_with_steel	Steel
Bearing_steel	Machine_parts_with_steel

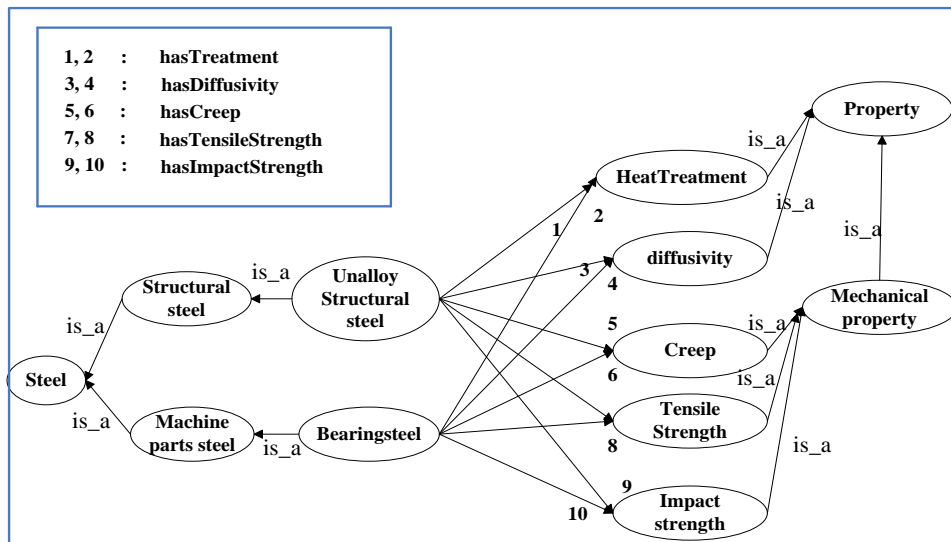


Figure 6. Relationships between Important Concepts (Part)

5. Design of Axioms and Rules in STSM

5.1. Design of Axioms

In STSM, the restrictive axioms A_r appears frequently in STSM, and it can be used to organize the relationships between these classes, and limit the domain and range of the object properties or data properties. The defined axioms A_d in the STSM is used to define concepts. For example, the Ferrite steel is a steel whose basic organizations includes ferrite, and these concepts and individuals which meet the definition will belong to the defined concept. We try to design axioms according to the following two aspects [42, 43]. Firstly, there is no classification about microstructure in the STSM, so axioms can be designed to classify steel according to microstructure. Secondly, different classification standards and guidelines should be considered to support international generality.

We have implemented the axioms for steel microstructure, other axioms are being designed. Some of the implemented defined axioms are given as follows.

Axiom 1. Axioms for Ferrite steel.

Ferrite_steel \equiv Steel \cup \exists hasBasicOrganization.Ferrite.

Axiom 2. Axioms for Dual-phase steel.

Dual-phase_steel \equiv Steel \cup ≥ 2 hasBasicOrganization.BasicOrganization.

Axiom 3. Axioms for Austenite steel.

Austenite_steel \equiv Steel \cup \exists hasBasicOrganization.Austenite.

Axiom 4. Axioms for Martensite steel.

Martensite_steel \equiv Steel \cup \exists hasBasicOrganization.Marstensite.

Ferrite_steel on the left of the equation in Axiom 1 is the defined concept, and the right part is made up of atomic concept steel and anonymous class, which means that *Ferrite steel* is a kind of steel that includes at least a ferrite organization. As shown in Figure 7, *Ferrite steel* has not sub-concepts before reasoning in the protégé 4.3. However, the results are revealed as Figure 8 after reasoning with Pellet [44,45], and *Ferrite steel* has 6 sub-concepts as shown in Table 3.

Thus, we know that these materials belong to *Ferrite steel*. Furthermore, the axiom 3 shows the definition of *Austenite steel*, and *Austenite steel* is the materials that at least a basic organization which is austenite. The axioms of *Ferrite steel* and *Austenite steel* are similar with the axioms of *Martensite steel* and *Dual-phase steel*. It's worth noting that we have designed above axioms and more axioms are being designed.

Table 3. The Sub-concepts of Ferrite Steel in STSM (inferred)

Parent of concept	Concept in STSM
Ferrite steel	Austenite_ferrite_stainless_steel
Ferrite steel	F+P (Ferrite and Pearlite) not_hardened_and_tempered_steel
Ferrite steel	Ferrite_heat_resisting_steel
Ferrite steel	Ferrite_pearlite_heat_resisting_steel
Ferrite steel	Ferrite_stainless_steel
Ferrite steel	Low_alloy_high_strength_structral_steel

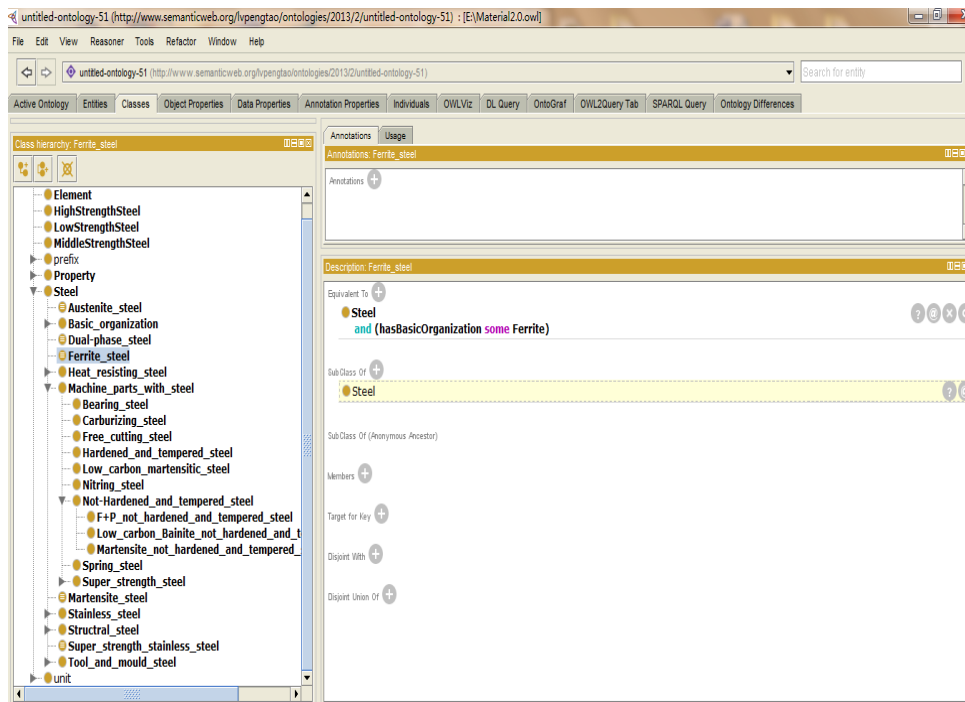


Figure 7. The Interface before Reasoning in Protégé 4.3

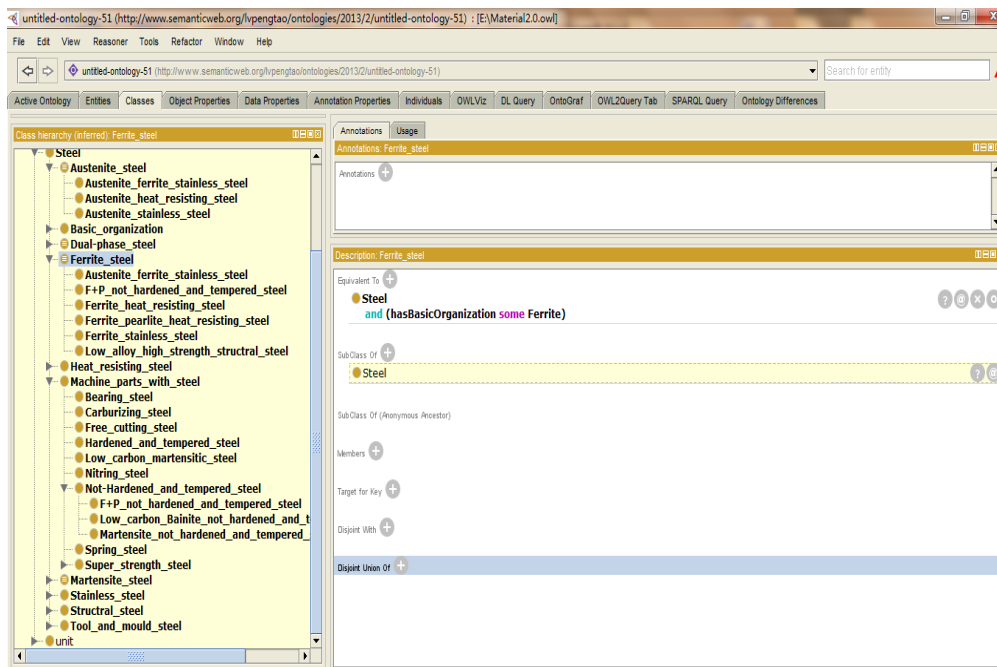


Figure 8. The Interface After Reasoning in Protégé 4.3

5.2. Design of Rules

Axioms have some limitations in representing knowledge. For example, high strength steel is the steel whose tensile strength is greater than 1400Mpa, and it would be difficult to be represented in axioms, because constraints in axioms always recognize a specific value and do not recognize value range. In other words, the axioms can identify 1400Mpa, but do not recognize the range which is greater than 1400Mpa. Hence, we should introduce rules [46,47,48] to STSM, which can represent knowledge that can not be represented by axioms. By making rules conforming to certain syntax and structure, new knowledge can be discovered by reasoning. The key issue of rule design is to find appropriate rules which are accepted by domain experts. This paper designs rules as follows, but they are not limited in these aspects, and more and more rules will be found with further research.

(1) Tensile strength. Steel will be classified into high strength steel or low strength steel according to tensile strength.

(2) Content of total alloy element. Alloy steel will be classified into high alloy steel, middle alloy steel and low alloy steel according to content of total alloy element.

(3) Stainless and corrosion-resisting steel. Stainless and corrosion-resisting steel is the steel whose Gr content is greater than 10.5%.

(4) Super strength stainless. If a kind of steel includes element Gr whose content value is greater than 10.5% and has tensile strength which is greater than 1400Mpa, then it is super strength stainless steel.

(5) The materials property may be predicted by relevant materials properties parameters.

In STSM, the first 4 rules belong to classification rules R_c , and the last rules belong to prediction rules R_p .

There are many rule languages, such as OWL [49], SWRL [50], RIF [2], Jena Rule [51], and the Jena Rule is used in STSM. Table 4 shows the rules of tensile strength. High strength steel is the steel whose tensile strength is greater than 1400Mpa, and low strength steel is the steel whose tensile strength is less than 700Mpa, and middle strength steel have tensile strength between 700Mpa and 1400Mpa. Table 5 gives the rules in super high strength stainless steel, and it means that super high strength stainless steel is that steel whose tensile strength is greater than 1400Mpa and Gr content is greater than 10.5%.

Table 4. Rules for Tensile Strength

Name	Rule
HighStrengthSteel	[HighStrengthSteel: (?x matowl :hasTensileStrength ?y) (?y matowl :hasUnit Mpa) (?y matowl :hasMinValue ?z) greaterThan(?z, 1400) ->(?x rdf:type matowl:HighStrengthSteel)]
LowStrengthSteel	[LowStrengthSteel: (?x matowl :hasTensileStrength ?y) (?y matowl :hasUnit Mpa) (?y matowl :hasMinValue ?z) lessThan(?z, 700) -> (?x rdf:type Matowl:LowStrengthSteel)]
MiddleStrengthSteel	[MiddleStrengthSteel: (?x matowl :hasTensileStrength ?y) (?y matowl :hasUnit Mpa) (?y matowl :hasMinValue ?z) lessThan(?z, 1400) greaterThan(?z, 700) ->(?x rdf:type matowl:LowStrengthSteel)]

Table 5. Rules in Super High Strength Stainless Steel

Name	Rule
SuperStrength StainlessSteel	[SuperStrengthStainlessSteel: (?x matowl :hasTensileStrength ?y) (?y matowl :hasMinValue ?z) greaterThan(?z, 1400) (?x matowl :hasChemicalCompostion?w) (?w matowl :hasElement matowl: Gr) (?w matowl :hasContentRatio ?f) greaterThan(?f, 0.105) ->(?x rdf:type matowl: SuperStrengthStainlessSteel)]

We develop the experimental prototype with Netbeans 7.3 and Jena for testing the rules. In Figure 9, the steel ontology tree is shown, and the rules can be selected. For example, we select the rule for low strength steel which is shown in Figure 9, and query condition “rdf: type” and “LowStrength” should also be selected, which means that we want to query the steel whose types are low strength steel. The corresponding SPARQL statement of the above query condition is **SPARQL 1**. Lastly, the desired query results are acquired in Figure 9. According to query results, we conclude that Q275, Q255, Q235, Q215 and Q195 belong to low strength steel, but their types are not low strength steel if we don’t choose any rules in the rule list.

SPARQL 1. SPARQL for low strength steel.

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SELECT ?x WHERE{
    ?x rdf:type matowl:LowStrengthSteel}
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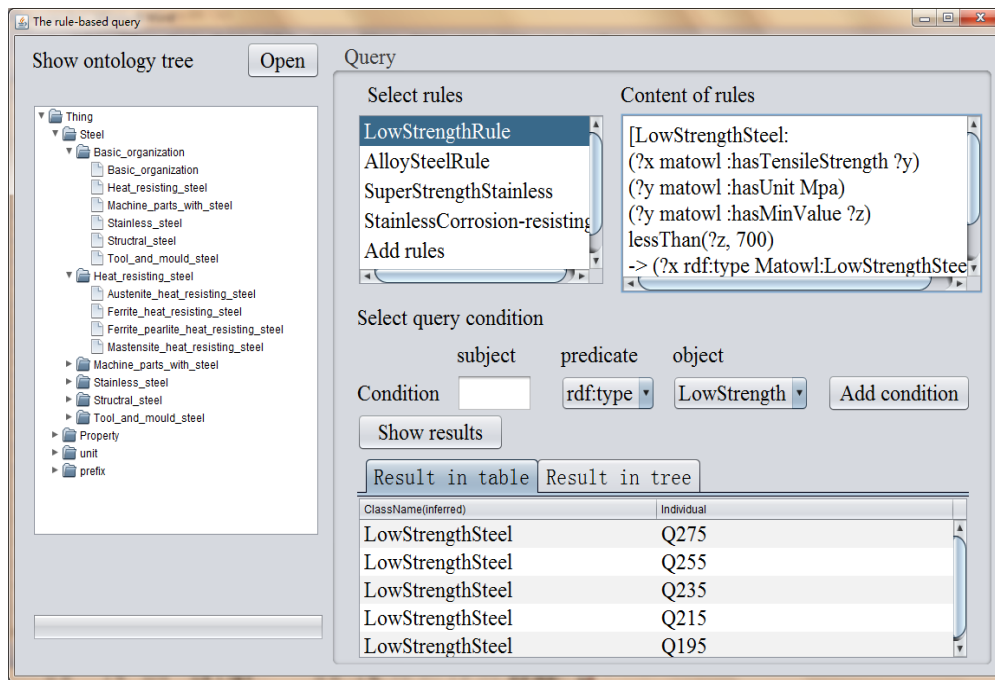


Figure 9. Query Results

6. Conclusion and Future Work

This paper discusses the construction process of a steel semantic model STSM with the consideration of the feature of materials knowledge. STSM covers the basic steel knowledge and can be used to integrate heterogeneous materials data. Further, we have developed some of the domain axioms and logic rules in STSM, which is sure to be helpful for discovering hidden materials knowledge by automatic reasoning. In future, STSM will be extended to the metal materials domain, so it can provide richer axioms and rules by elaborate analysis of materials domain knowledge. Besides, on the basis of STSM, we will populate the STSM with materials data from open data source to form a richer materials knowledge base.

Acknowledgements

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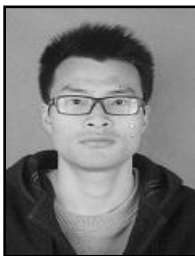
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