DEFINITION OF A WEB ONTOLOGY FOR DESIGN-ORIENTED MATERIAL SELECTION

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ABSTRACT

A standardized data schema for material properties in XML is under development to establish a common and exchangeable expression. The next stage toward the management of knowledge about material usage, selection or processing is to define an ontology that represents the structure of concepts related to materials, e.g., definition, classification or properties of material.

Material selection for designing artifacts is a process that translates required material properties into material substances, which in turn requires a definition of data analysis and rules to interpret the result. In this paper, an ontology structure to formalize this kind of process is discussed using an example of the translation of creep property data into design data.

Keywords: Knowledge Management, Material Science, Ontology

1 INTRODUCTION

XML is widely accepted as the standard infrastructure for data exchange on the Internet (Boucelma, O., Castano, S., Goble, C., Josifovski, V., Lacroix, Z. & Ludäscher, B., 2002) and MatML is being developed as a standard data schema for material data exchange. MatML (MatML) makes heterogeneous databases and applications interoperable, but it does not represent the meanings of material data. In order to formalize and share knowledge about materials, the definition of material properties, material processing or usage, higher level standardization is required. (Figure 1)

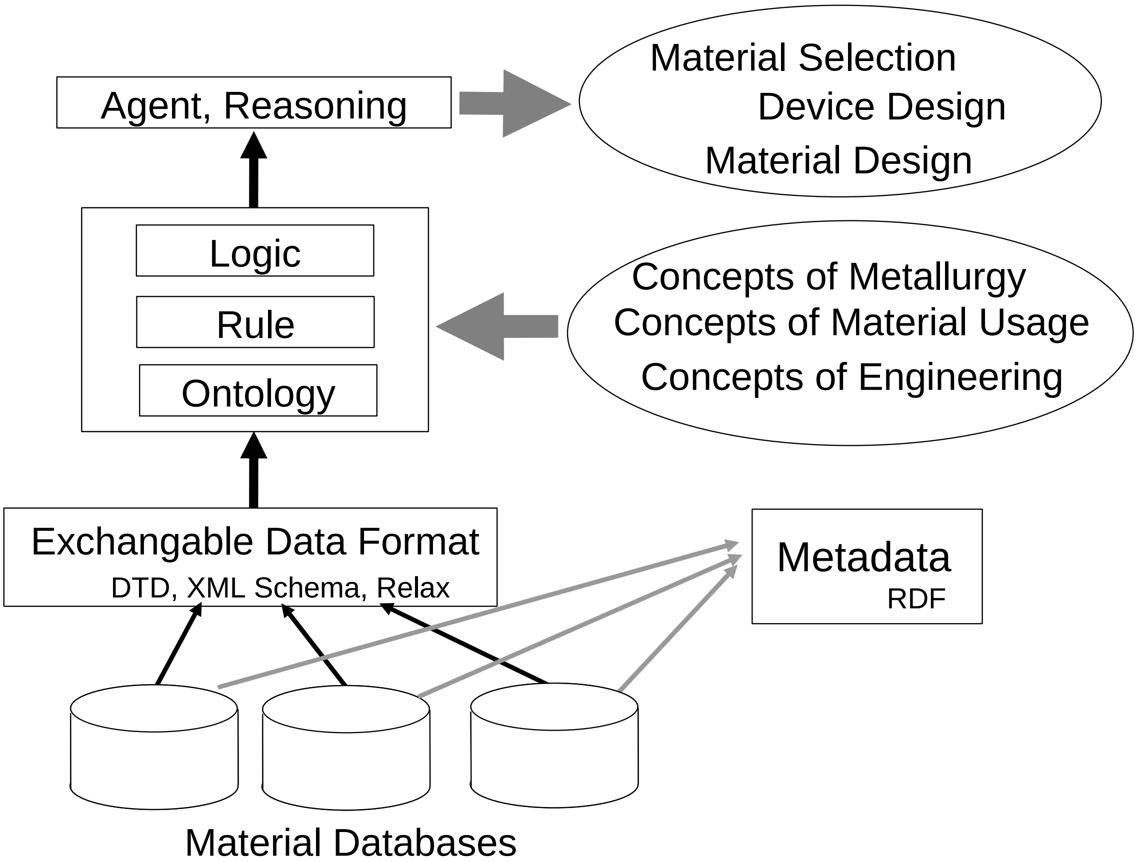

Figure 1. Material databases and Semantic Web technology

The Semantic Web is an Internet based re-engineering of 1980's knowledge technology which enables Internet-wide knowledge sharing. (Berners-Lee, T., Hendler, J. & Lassila, O., 2001) It has a layered structure, and standardization proceeds from lower layer to upper layer. Lower layers, XML and XML Schema for data schema definition, RDF - Resource Definition Framework - for metadata and OWL - Web Ontology Language - for ontology representation are already standardized. Upper layers, rules, logic framework and proof are now under development.

The current focus is the ontology layer. Standard ontology definition have been proposed in many areas to share meanings of concepts in each domain (The Gene Ontology Consortium, 2000, Miller, J. A., Baramidze, G. T., Sheth, A. P. & Fishwick, P. A., 2004), but no standard ontology for concepts about materials is available. Material science is so large and concerns a wide dimensional scale, micro to macro, together with many kinds of materials, properties and applications. (Westbrook, J. H., 2003) As an illustration of ontology development in material science, this paper focuses on the concepts related to the creep properties of an alloy.

Creep is a process of slow deformation of a solid and is an important factor to control the lifetime of devices especially at high temperatures. (Dieter, Jr., G. E., 1961) Design parameters are derived from experimental data with data analysis procedures which are described in computer programs and documents. An ontology definition schema for data processing on a semantic web is presented.

2 A MATERIAL TAXONOMY FROM A THESAURUS

The dictionary definition of ontology is "a branch of philosophy that deals with the nature of existence", but the use in computer science is different. (Chandrasekaran, B., Josephson, J. R. & Benjamins, V. R., 1999) Some AI researchers use it as a concept that enables intelligent activity, but in this paper, we use it in the most practicable meaning, i.e. objects, concepts or other entities about some knowledge and relationships among them. (Noy, N. F. & Hafner, C. D., 1997, Uschold, M. & Gruninger, M., 2004)

A thesaurus is regarded as a subset of ontology. (Wielinga, B. J., Schreiber, A. Th., Wielemaker, J. & Sandberg, J. A. C., 2001) As a first step to create an ontology of material science, we tried to derive an ontology definition from a material thesaurus, which includes over 6,000 unique entries, based on the ASM metallurgical thesaurus (Anton, G. J., Bullard, S. R., Chang, M. S., Donaldson, C., Finical, M.P., Jones, M. S., et. al., 1996) as improved and converted into digital form by Fujita, et al. The following five types of relationships are used in this thesaurus.

BR - BRoader terms (generally BT)
NA - NArrower terms (generally NT)
RT - Related Terms
UF - Used For terms
JP - JaPanese translation

Figure 2 shows the structure of the subtree that begins from the term "alloy". The solid lines shows BR and NA relations. The dashed lines show RT relations. The term "metal" is a broader term of "alloy". The term "alloy" has narrower terms, which specify material type or usage, such as "brazing alloy", "heat resistant alloy", "dispersion hardening alloy" or "magnetic alloy". On the other hand, properties of materials, such as "phase diagram", "composition" or "crystal structure" are connected to "alloy" with an RT relation.

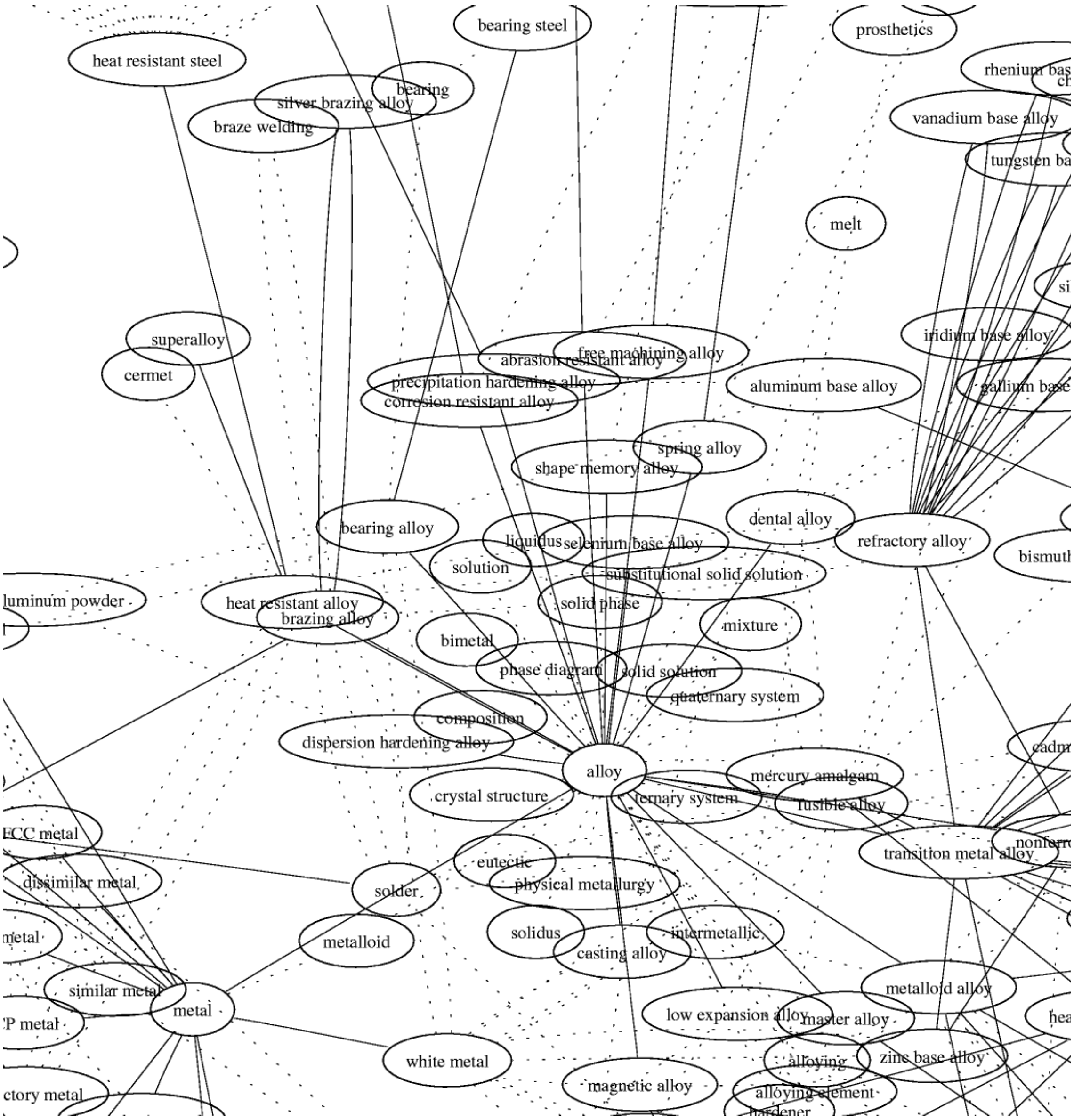

Figure 2. Network structure of a material thesaurus subtree which begins from the term “alloy”

We found that the thesaurus includes rich vocabulary about material taxonomy, but it is not enough to describe the flow of material data analysis. For example, the subtree of "creep", which is the narrower term of "mechanical property", is shown in Figure 3. The subtree is adequate to classify a material based on creep properties and describe related metallurgical concepts, but not to describe how to derive "creep strength" from creep experiment data or how creep data is used in the design process for a device.

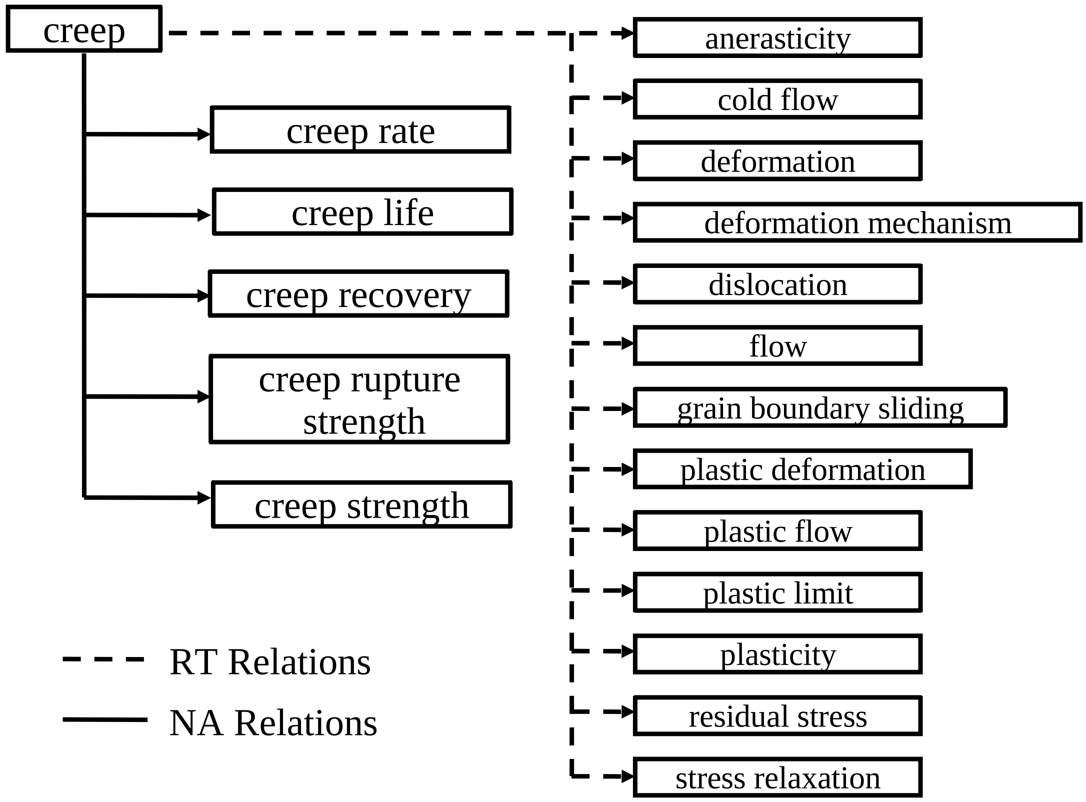

Figure 3. Entries in a metallurgical thesaurus relate to the entry "Creep"

3 A CONCEPT MAP FOR CREEP PROPERTIES

The creep property of a material is an important parameter for material selection for high temperature device design. Figure 4 shows related concepts for the derivation of design parameters from a creep data sheet. (National Institute for Materials Science, Japan, 2002) In this chart, the upper left side shows the taxonomy of materials which derived from the thesaurus of metallurgical terms. (Yoshizu, H., Yamazaki, M. Halada, K, Fujita, M. & Nakata, T., 2004). These relationships, however, are useless for material selection based on creep databases, as they do not contain the relationships between experiment data and creep properties.

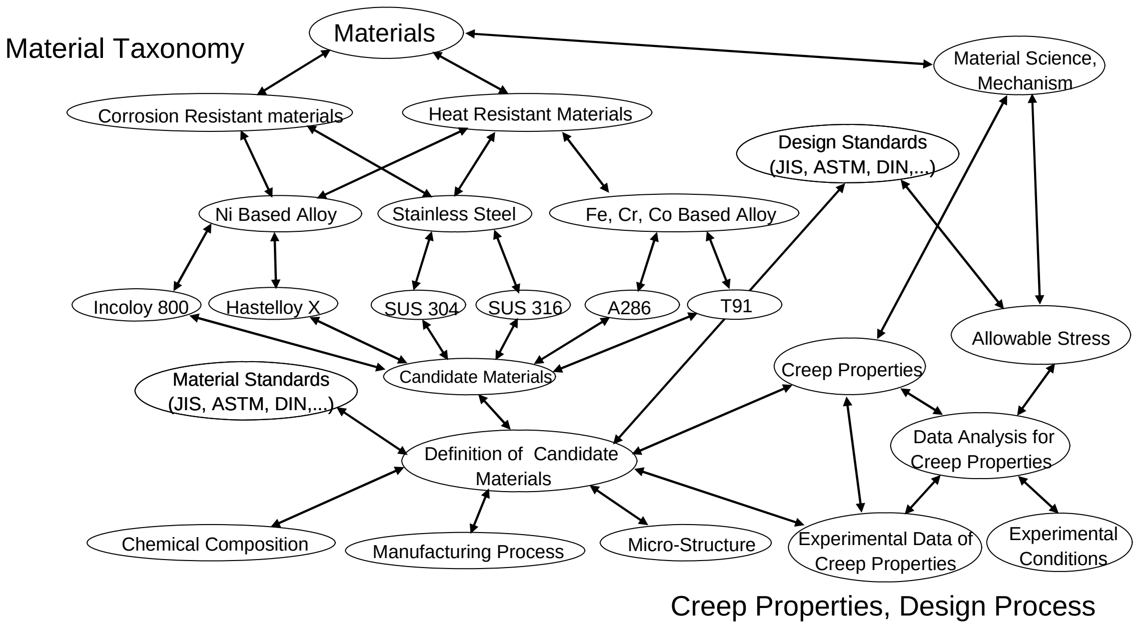

Figure 4. Relations of concepts related to creep properties of materials

The lower right area describes the relation of creep properties and other concepts, as organized from the viewpoint of device/plant design. The definition of candidate materials is derived from the comparison between the result of an analysis of experimental data and required specification.

The creep data analysis procedure is shown in detail in Figure 5. Creep experiment data are analyzed and extrapolated to give a design curve, which in turn enables the estimation of material lifetime under the specified conditions. Also, design curves enable specification of the definition of candidate materials, and an existent material can be selected based on this definition.

In this procedure, two regression curves, "Creep Curve" and "Creep Rupture Curve" are the key concepts for translating experimental creep data into a design curve. These two regression curves are fitted with a non-linear regression method based on metallurgical experiments and theories. The "Creep Rupture Curve" illustrates the creep behavior of a material as a function of time and temperature. The "Design Curve" is given by extrapolation based on metallurgical knowledge.

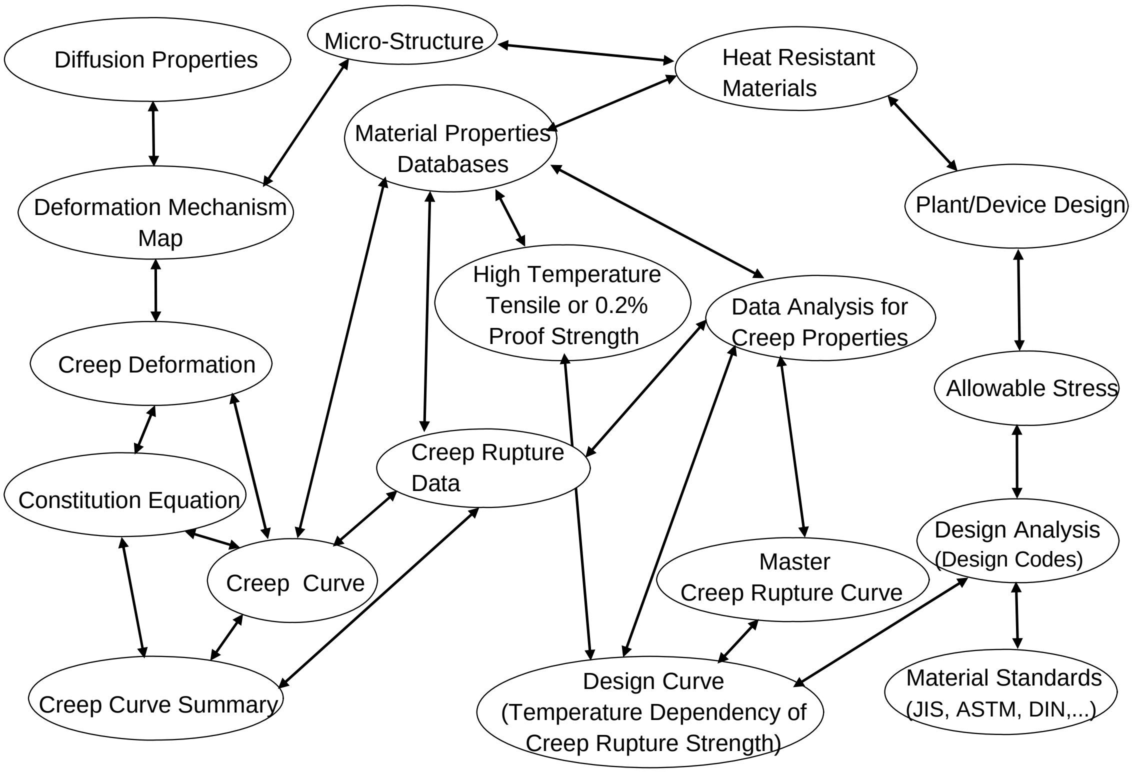

Figure 5. Standard procedure to derive a design curve from a creep data sheet

4 AN ONTOLOGY DEFINITION FOR MATERIAL DATA ANALYSIS

In order to formalize and manage the knowledge, as described in the previous section, with a semantic web framework, concepts are allocated into each layer as shown in Table 1. A standard material properties data schema, MatML is defined in the lowest layer, XML Schema. MatML does not, however, define creep or other physical property names. A reference schema definition of creep test data in an XML Schema is shown in Figure 6. The complexType "CreepTest" includes one or more data points, and each point has the complexType "CreepData". The attribute "object," which specifies the specimen, is defined as the type "materialspec," as defined in MatML.

Table 1. An application of a Semantic Web framework to data and knowledge of material science

Layer	Material Knowledge
Rules, Logics,..	Usage of analysis methods; design standards
Ontology (OWL)	Taxonomy of material; definition of data analysis methods
Metadata (RDF)	Metadata description of material databases
Schema (XML Schema)	Material properties data schema (MatML)

```
<xsd:complexType name="CreepTest">
  <xsd:sequence>
    <!-- one or more experimental data point -->
    <!-- CreepData is the other complexType -->
    <xsd:element name="data" type="CreepData" minOccurs="1"/>
  </xsd:sequence>
  <!-- specification of material -->
  <xsd:attribute name="object" type="matml:materialspec"/>
  <!-- experimental condition -->
  <xsd:attribute name="temperature" type="xsd:float"/>
  <xsd:attribute name="pressure" type="xsd:float"/>
</xsd:complexType>
```

Figure 6. A reference data schema definition of creep test data

The second lowest layer RDF is used to describe metadata of material databases, e.g., definition of the relations of data fields. Generally, ontology defines the taxonomy of a concerned domain, in this case materials. We decided that the definition of data analysis methods for creep data should be described in this layer. Knowledge about data analysis methods are written in computer programs as statements for computation, database access or branch condition, but a declarative description such as an ontology is easier to verify, reuse and read than the program statements in a procedural description.

The creep curve is the result of a non-linear regression analysis of experimental creep data, a set of measured strains over time, with regression equation given by metallurgical theory. The creep rupture curve is a summary of several individual creep curves at different temperatures. Figure 7 describes the process for treating creep curves and the creep rupture curve as ontology classes. Knowledge about how to interpret or evaluate the curves or how to extrapolate the data are left to higher rule and logic layers of the Semantic Web.

The major difference between a schema and an ontology is the capability of inference. Inference engine can be applied to drive data analysis. To show the data analysis process by an inference engine with an ontology definition, a simplified definition, is written "CreepCurve" in OWL Web Ontology Language (Smith, M. K., Welty, C. & McGuiness, D. L., 2004), is shown in Figure 8. Figure 9 shows the same data structure as a diagram.

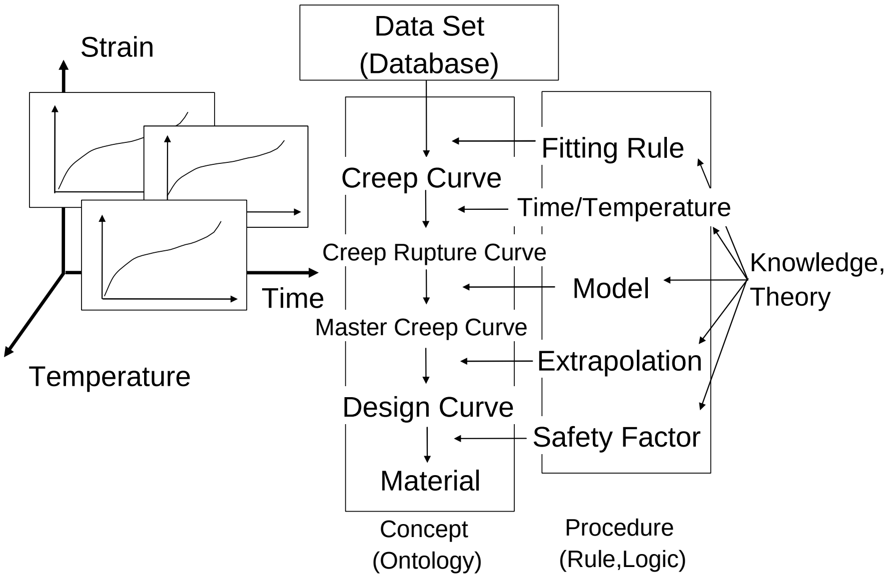

Figure 7. A flow of creep data analysis with Ontology and Rule

```
<owl:Class rdf:ID="CreepCurve">
 <rdfs:subClassOf>
   <owl:Class rdf:ID="regression:RegressionCurve"/>
 </rdfs:subClassOf>
</owl:Class>

<owl:ObjectProperty rdf:ID="Source">
  <rdfs:domain rdf:resource="#CreepCurve"/>
 <rdfs:range rdf:resource="&material;CreepTest"/>
</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID="Coefficients">
 <rdfs:domain rdf:resource="#RegressionCurve"/>
 <rdfs:range rdf:resource="&regression;coefficient"/>
</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID="RegressionEquation">
 <rdfs:domain rdf:resource="#RegressionCurve"/>
 <rdfs:range rdf:resource="&regression;equation"/>
</owl:ObjectProperty>

<owl:ObjectProperty rdf:ID=”Algorithm”>
 <rdfs:domain rdf:resource=”#RegressionCurve”/>
 <rdfs:range rdf:resource=”&regression;algorithm”/>
</owl:ObjectProperty>

<owl:Class rdf:ID="RegressionCurve">
 <rdfs:subClassOf>
   <owl:Restriction>
     <owl:onProperty rdf:resource="#Coefficients">
       <owl:minCardinality rdf:datatype="&xsd;int">1</owl:minCardinality>
     </owl:onProperty>
   </owl:Restriction>
  </rdfs:subClassOf>
</owl:Class>
```

Figure 8. A sample definition of a creep curve ontology

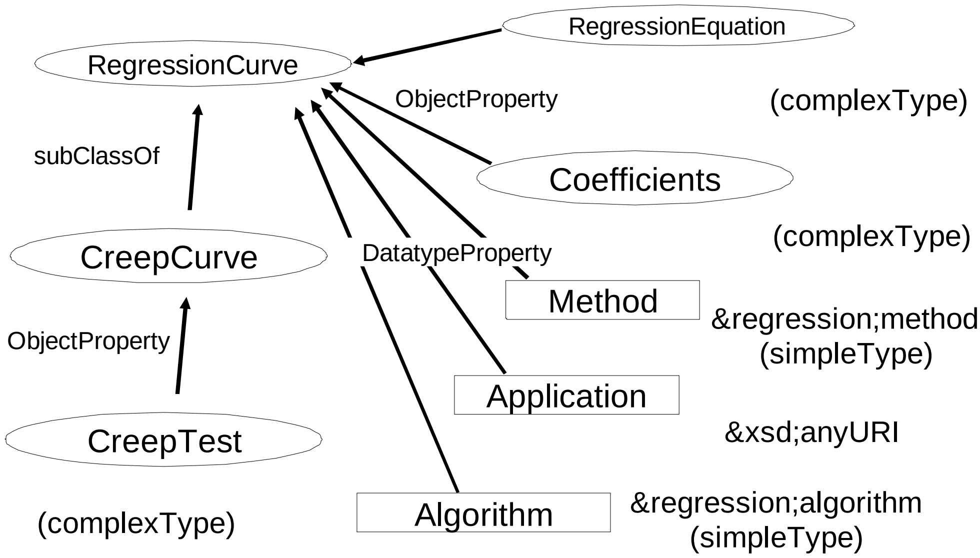

Figure 9. Diagram of a creep curve ontology definition

In this definition, "CreepCurve" is a subclass of “RegressionCurve” (line 1-5) and inherits the properties "Coefficients", "RegressionEquation" and “Algorithm” from "RegressionCurve" (line 13-26). Also "CreepCurve" has a property named "Source," which includes "CreepTest" data (line 7-11). When "CreepCurve" is instantiated with values of "Source" and "RegressionEquation", an inference engine can deduce how the value of "Coefficient" can be calculated with “Algorithm”.

Rules - for example to select an appropriate regression algorithm for a given regression equation or an appropriate regression equation for a specified material type - are left to the upper layer. A Rule Language for a Semantic Web is now under development, and it will be a few more years before standardization.

5 CONCLUSION

In order to formalize and manage knowledge about materials with semantic web technology and tools, it is necessary to decide which kind of knowledge should be mapped into which layer of the semantic web architecture. The basic structure of a material taxonomy in an ontology layer can be derived from a material thesaurus, as has been demonstrated. Also, a creep data analysis procedure can be expressed as an ontology with declarative description by using the Web Ontology Language. By using OWL, knowledge about creep data analysis can be integrated with material databases via the standardized XML schema data representation.

Data analysis procedures are basic to science and technology. The library of such basic procedure definitions is an important infrastructure of a scientific application of a semantic web. Also a further detailed definition of material properties over MatML is required to access material data from upper layer definitions of material knowledge.

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