Formalization of material property data analysis with web ontology

Toshihiro Ashin[1] and Hiroshi Yoshizu[2]

[1] Faculty of Regional Development Studies, Toyo University, 1-1-1 Izumino, Itakura-Cho, Oura-Gun, Gunma-Ken, 374-0193, Japan, ashino@acm.org
[2] National Institute for Materials Science, 1-2-1 Sengen, Tsukuba-City, Ibaraki, 305-0047, Japan, yoshizu.hiroshi@nims.go.jp

Abstract. A standardized data schema for material properties in XML is under development to establish common and exchangeable data expression. The next stage toward knowledge management about material usage, selection or processing is to define an ontology which represents the structure of concepts relating to materials, e.g., taxonomy, analysis or properties of materials.
Material selection for designing artifacts is a process of translating required material properties into a specific material substance. In order to manage knowledge of this process, definitions and rules of data analysis should be formalized in computer readable format. In this paper, an ontology structure for design process is discussed using the example of the creep property of materials.

1 Introduction

XML is widely accepted as the standard infrastructure for data exchange on the Internet [1] and MatML is developed as an standard data schema for the material data exchange. MatML [2] 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, standardized definitions for higher level concepts are required.(Fig. 1)

Semantic Web is an Internet based re-engineering of 1980's knowledge technology which enables Internet-wide knowledge sharing. [3] 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.

Standard ontology definition have been proposed in many areas to share meanings of concepts in each domain [4, 5] but no standard ontology for concepts about materials is proposed.

Material science is so huge and concerns a wide dimensional scale, micro to macro, together with many kinds of materials, properties and applications. [6] Therefore, this paper focuses on the concepts related to creep property of an

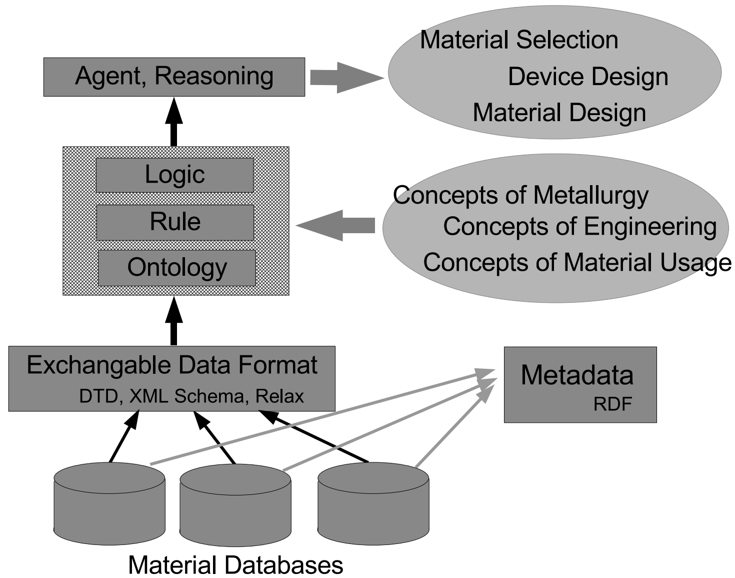

Fig. 1. Material Databases and Semantic Web Technology

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. [7] An ontology definition schema and usage to formalize the description of creep property and creep data analysis for designing high temperature device is presented.

2 A Concept Map for Creep Properties

The creep property of a material is important parameter for material selection for high temperature device design. Fig. 2 shows related concepts for derivation of design parameters from creep data sheet. [8] In this chart, the upper left side shows the taxonomy of materials which derived from the thesaurus of metallurgical terms. [9, 10] But these term relationships are useless for material selection, since they are not based on creep properties of materials.

The lower right area describes the relations of creep properties and other concepts which are organized from the viewpoint of device/plant design. 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 Fig. 3. [11] Creep experiment data is analyzed and extrapolated to give a design curve which enables to estimate the lifetime of a material under the specified conditions. Also, design curves enable to specify the definition of candidate materials and an existent material is selected based on the 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.

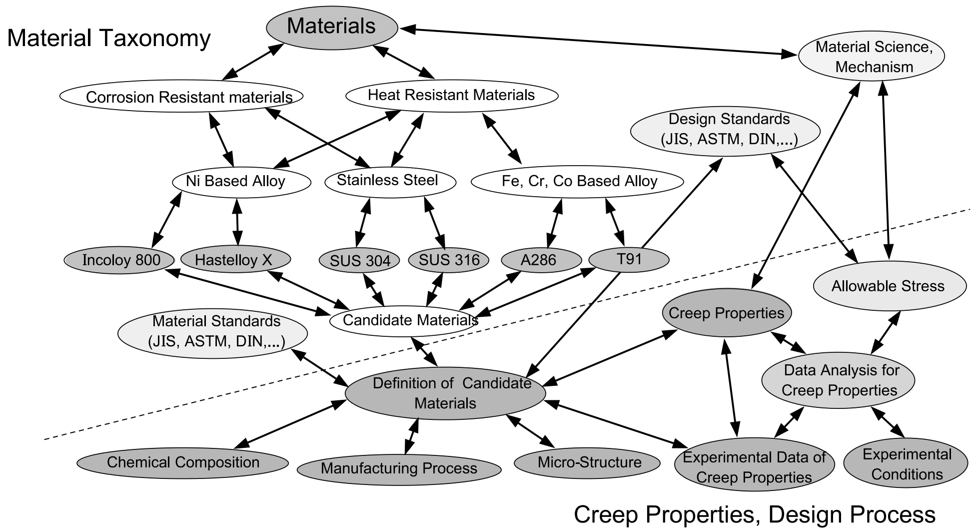

Fig. 2. The Structure of Concepts Related to Creep Properties of Materials

These two regression curves are fitted with non-linear regression method to appropriate regression equations which are based on metallurgical experiments and theories. "Creep Rupture Curve" illustrates the creep behavior of a material as a function of time and temperature. "Design Curve" is given by extrapolation based on metallurgical knowledge.

3 An Ontology Definition for Material Data Analysis

In order to formalize and manage knowledge which described in the previous section with semantic web framework, concepts are allocated into each layer as shown in Table 1. Standard material properties data schema, MatML is defined in XML Schema. But MatML does not define creep or other physical property names.

A reference "CreepTest" data schema definition which is written in XML Schema is shown in Fig. 4. The complexType "CreepTest" includes one or more data points which is defined as the other complexType "CreepData", the attribute "object" which specifies the specimen, has the type "materialspec" which is defined in MatML.

The Upper layer, RDF is used for describe metadata of material databases, e.g. definition of the relations of data fields. Generally, ontology defines the taxonomy of concerned domain like material in this case. Additionally the definition of data analysis methods for creep data analysis is described in this layer. Knowledge about data analysis methods are buried in computer programs as procedure, e.g. statements for computation, database access or branch condition.

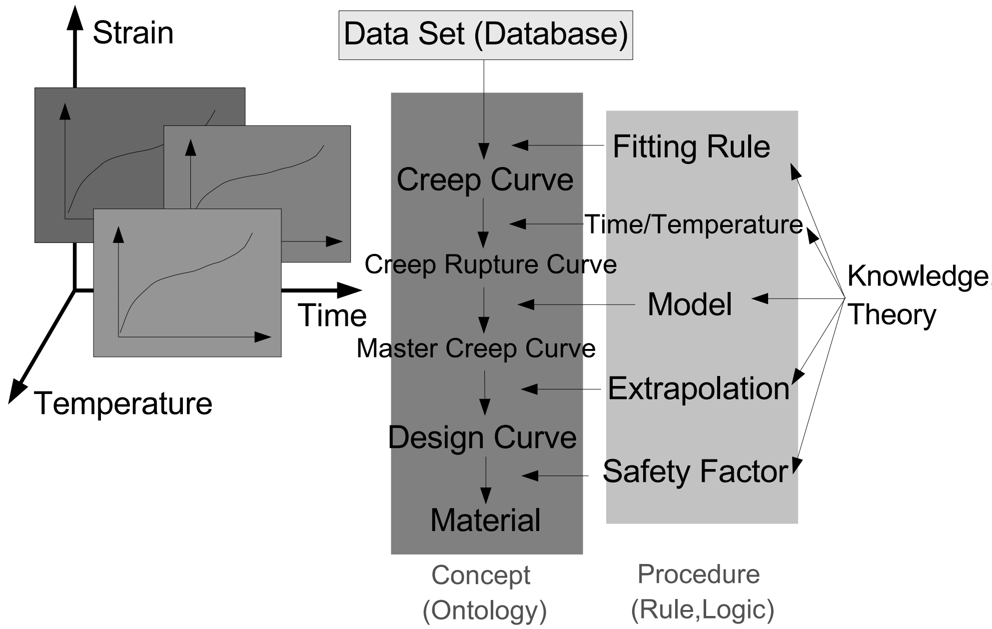

Fig. 3. Standard Procedure to Derive Design Curve from Creep Data Sheet

Table 1. An application of Semantic Web Framework to Data and Knowledge of Material Science

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>
```

Fig. 4. A reference data schema definition of creep test data

But declarative description like ontology is easier to verify, more reusable and readable than procedural description like program statements. The major difference between schema and ontology is the capability of inference. Inference engine can be applied to drive data analysis.

To show the data analysis process by inference engine with ontology definition, simplified definition of “CreepCurve” in OWL, Web Ontology Language [12], is shown in Fig. 5.

In this definition, “CreepCurve” is a subclass and inherits properties “Coefficients” and “RegressionEquation” from the class “RegressionCurve”. Also “CreepCurve” has a property named “Source” which includes “CreepTest” data. When instantiate “CreepCurve” with values of “Source” and “RegressionEquation”, inference engine can deduce how the value of “Coefficient” can be calculated.

Rules, for example to select appropriate regression algorithm for given regression equation or appropriate regression equation for specified material type, is left to upper layer. Rule Language for Semantic Web is now under development [13, 14] and it will take few more years before standardization.

4 Conclusion

Creep data analysis procedure can be expressed with declarative description by using OWL, Web Ontology Language in a natural manner. And by using OWL, knowledge about creep data analysis can be integrated with material databases via the standardized XML Schema data representation. Basic data analysis procedure is common in science and technology and the standardization of its definition is important to e-science.

```
<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: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>
```

Fig. 5. A part of ontology definition of creep curve

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