MatML: XML for Information Exchange with Materials Property Data

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ABSTRACT
This paper describes the development and use of MatML, the Materials Markup Language. MatML is an emerging XML standard intended primarily for the exchange of materials property information. It provides a medium of communication for users in materials science and related fields such as manufacturing and aerospace. It sets the stage for the development of semantic web standards to enhance knowledge discovery in materials science and related areas. MatML has been used in applications such as the development of materials digital libraries and analysis of contaminant emissions data. Data mining applications of MatML include statistical process control and failure analysis. Challenges in promoting MatML involve satisfying a broad range of constituencies in the international engineering and materials science community and also adhering to other related standards in web data exchange. These issues are being addressed through the development of a good ontology, the automation of format conversions and possible schema extensions. MatML aims to be a lingua franca for data exchange in materials science and its broader horizons.

Categories and Subject Descriptors
H.3.7 [**Information Storage and Retrieval**]: Digital Libraries – *Dissemination, Standards, User Issues.*

General Terms
Documentation, Standardization

Keywords
Information Exchange, Data Mining, Semantic Web

1. INTRODUCTION
XML, the eXtensible Markup Language is today a widely accepted standard for storage and exchange of information. It serves a twofold purpose of providing a data model for storing information and a medium of communication for exchanging information over the worldwide web [29].

Domain-specific markup languages are often defined within the context of XML to serve as the means for storing and exchanging information in the respective domains. Some examples of such markup languages include [14, 9]:

- AniML: Analytical Information Markup Language
- ChemML: Chemical Markup Language
- femML: Finite Element Modeling Markup Language
- MathML: Mathematics Markup Language
- ThermoML: Thermodynamic Markup Language
- WML: Wireless Markup Language
- UnitsML: Units Markup Language

These XML-based languages enable the storage, retrieval and display of information using a non proprietary format [14, 29]. They describe the given domain in an understandable language that is common to its members and interested parties, thus enabling effective information exchange [9].

It was realized by materials scientists that there was a need for a common medium to exchange materials data of various types in different organizations across the globe [14]. Languages such as HTML [8] have non-descriptive fixed tag-sets. Hence there was a need for a language with a more intelligible and malleable structure, a descriptive nature and extensibility [12]. This motivated the development of MatML, the Materials Markup Language.

The main goal of MatML was thus to serve as a medium of communication for storing and exchanging materials properties information across organizations worldwide [12, 9]. This is illustrated in Figure 1 [14].

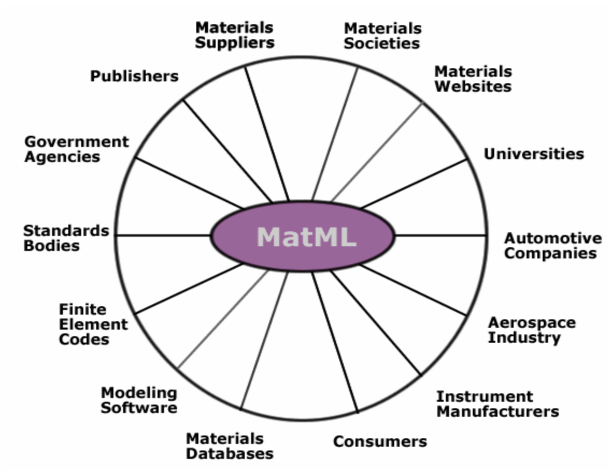

Figure 1: Goal of MatML – Medium of Communication

More specifically, MatML was created to equip the materials data marketplace with the following [14]:

- Common materials data exchange format
- Non-proprietary "Esperanto"
- Direct program to program interoperability
- Flexible, extensible markup language

The MatML effort was pioneered at NIST, the National Institute of Standards and Technology [16]. Its development began in October 1999. Today it has expanded to the MatML Coordination Committee [14], spearheaded by ASM International, the Materials Information Society [3], and comprising a consortium of experts from academia and industry.

Standardization of MatML is currently governed by OASIS, the Organization for the Advancement of Structured Information Standards [18]. We discuss the details of MatML in the sections to follow.

Section 2 of this paper explains development of MatML. Section 3 gives examples of real-world success stories with MatML. Section 4 presents an overview of the data mining applications envisaged for MatML promoting its further use. Section 5 outlines the challenges encountered in MatML at present and the ongoing work to address them. Section 6 states the conclusions.

2. DEVELOPMENT OF MATML

2.1 Overview of the MatML Schema

MatML was originally defined using a DTD (Document Type Definition) in April 2000 [14] and was later enhanced into a schema in December 2002 [21, 5]. The present version of the schema (MatML version 3.1) [5] was created in October 2004. We present a brief description of this schema. The hierarchy of elements in this schema is as follows. There are several levels of nesting of which we show the first 3 in the schema snapshot in Figure 2 [5].

```
<MatML_Doc>
    <Material>
        <BulkDetails> ...
        </BulkDetails>
        <ComponentDetails> ...
        </ComponentDetails>
        <Graphs> ...
        </Graphs>
        <Glossary> ...
        </Glossary>
    </Material>
    <Metadata>
        <AuthorityDetails> ...
        </AuthorityDetails>
        <DataSourceDetails> ...
        </DataSourceDetails>
        <MeasurementTechniqueDetails> ...
        </MeasurementTechniqueDetails>
        <ParameterDetails> ...
        </ParameterDetails>
        <PropertyDetails> ...
        </PropertyDetails>
        <SourceDetails> ...
        </SourceDetails>
        <SpecimenDetails> ...
        </SpecimenDetails>.
        <TestConditionDetails> ...
        </TestConditionDetails>
    </Metadata>
</MatML_Doc>
```

Figure 2: Snapshot of the MatML Schema

The root of the MatML schema is the *MatML_Doc* element which declares the content model for a MatML document. Content models explain the relationships of the element and its child elements. Each *MatML_Doc* must have one or more *Material* elements [5].

Other than that there is the *Metadata* element with explanations of the data sources, properties, measurement techniques, specimens, and parameters referenced when materials property data is coded with other elements. The *Metadata* element may occur once or not at all [5].

The individual elements within the Material elements are descriptive tags on the material properties. Among these the *Graph* element stores two-dimensional graphics while the *Glossary* element has a definition of the terminology. The elements within *Metadata* store information pertinent to material details, e.g., parameters and specimens [5].

Details on the elements in *MatML_Doc* and tags within each element are beyond the scope of this paper. More information can be found in the detailed MatML schema [5]. Figure 2 shows an example of storing materials property data by using the MatML schema [5].

```
<Material>
    <BulkDetails>
        <Name>Carpet 2_HOD93</Name>
        <Class>FLOOR MATERIALS</Class>
        <Subclass>Carpet- synthetic fiber</Subclass>
        <Specification authority="NAICS">31411</Specification>
        <Notes>Residential; Polypropylene primary backing;
          Polyurethane secondary backing; 100% Nylon fiber;
          cut pile construction; back dyed; roll form; over pad installation
        </Notes>
    </BulkDetails>
    <ComponentDetails>
        <Name>2,6-Di-tert-butyl-4-methylphenol</Name>
        <Specification authority="CASN">126-37-0</Specification>
        <PropertyData property="pr4" technique="m1" source="ds1"
         specimen="s1" test="t1">
        <Data format="float">214</Data>
        <Uncertainty>
            <Value format="float">20.5</Value>
            <Units name="ug/m^2/h">
                <Unit><Name>ug</Name></Unit>
                <Unit power="-2"><Name>m</Name></Unit>
                <Unit power="-1"><Name>h</Name></Unit>
            </Units>
        </Uncertainty>
        <ParameterValue parameter="p10" format="float">
            <Data>24</Data>
        </ParameterValue>
        <ParameterValue parameter="p12" format="text">
            <Data>0.0013 - 0.01</Data>
        </ParameterValue>
        </PropertyData>
        <Notes>Molecular weight is 198 amu.</Notes>
    </ComponentDetails>
</Material>
```

Figure 3: Example of Data Storage using MatML

2.2. Advantages of MatML

The development of MatML has been an important contribution to the field of materials science and presents an interesting application of XML [14, 29].

In general, MatML offers the following benefits [21].

- Simplicity
- Understandability
- Flexibility
- Extensibility
- Cost Effectiveness

It is simple and understandable because documents in MatML can be read and written without difficulty by materials engineers and scientists. Moreover, the documents can be readily transmitted over a network. Also, MatML can be very easily used with state-of-the-art programming languages [11].

MatML is flexible in the sense that it can be applied to different materials from various sources. Several types of materials data can be exchanged. This includes chemical, mechanical, micro-structural and nano-structural data [11]. Materials with multiple components, such as a composite, e.g., multi-layer SiC-reinforced metals can be accommodated.

The extensibility of MatML refers to its ability to include other markup languages through the use of namespaces. Examples of such languages are ChemML, MathML, ThermoML and aniML. Namespaces are helpful because they permit the use of existing conventions instead of re-invention or duplication [11].

MatML is cost-effective since it avoids repetitive programming in exchanging data across organizations. In addition, it facilitates the development of user-friendly software tools for data conversion. It also simplifies the installation of new incoming transactions [11].

3. MATML SUCCESS STORIES

3.1 Development of a Materials Digital Library

A digital library is an online repository of information analogous to a physical library. Such online repositories facilitate the dissemination of knowledge among students, educators, and scientists [1]. The National Science Foundation (NSF) [17] put forth an effort called the NSF Materials Digital Library (MatDL) [13]. The organizations involved in this effort were the Massachusetts Institute of Technology (MIT), Kent State University (KSU) and University of Michigan (U-M). This MatDL adapted open source tools such as an image gallery and a version control system to serve materials science users [1]. MatML was found useful for this purpose.

A web-based MatML grapher [2] was developed that facilitated the comparison of selected materials properties of approximately 80 materials stored using MatML. The MatML grapher added value in an educational context by permitting users to visualize real property data in order to support decisions on selection of materials for process optimization. This grapher formed a part of the submission tool to the MatDL. It prompted users for domain-specific data, and automatically generated and attached keywords and editable descriptions.

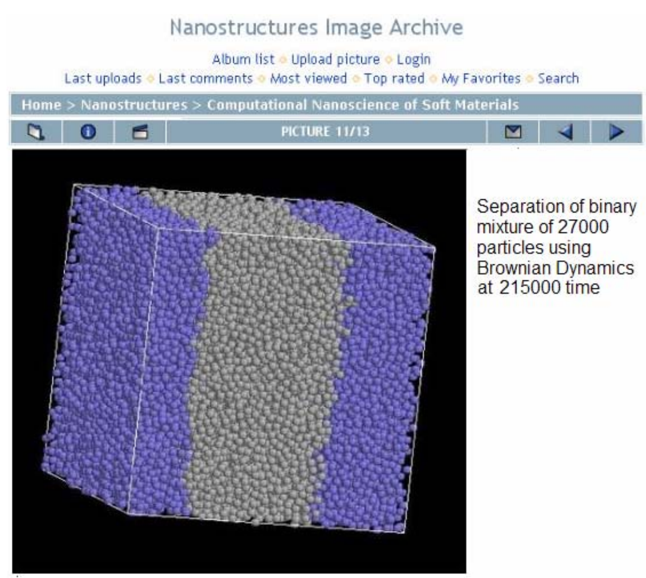

Figure 4: An Image in the MatDL Nanostructure Gallery

This tool was assimilated into the regular workflow of researchers in U-M [2]. It helped to visualize, for example, nanostructure images facilitating at-a-glance access to such information online.

Figure 4 illustrates an example of such an image stored in the MatDL nanostructure image gallery [2, 13].

A thorough study was done to find out whether digital libraries benefit from tools that integrate the libraries into the workspaces of researchers [1, 2]. Several roles that digital libraries can play were investigated such as supporting virtual laboratories, developing markup language applications, and building tools to capture metadata [1, 2]. MatDL set the stage for an MIT virtual laboratory experience. Student surveys indicated positive opinions on the role of MatDL in virtual laboratories and in fulfilling other educational objectives.

Another survey proved that a virtual laboratory could be as effective as a physical laboratory in meeting some learning goals. The tools are being enhanced to make submission to MatDL even easier and to minimize redundancy. Such services provided by MatDL aim to be a part of the users' virtual laboratory or workspace [13].

MatDL [13] is part of the National Science Digital Library project and is supported by National Science Foundation (NSF) [17] grant DUE-0333520 and National Institute of Standards and Technology grant 70NANB3H1079.

3.2 Management of Building Processes Data

Indoor air quality (IAQ) models for estimation of building contaminant concentrations generally need data from users pertaining to contaminant source strengths and transport mechanisms [6]. It was found that much of this input though available was not compiled in an easily accessible source. Hence users often needed to supply their own data.

This issue was addressed through an initiative that involved the use of MatML for storing contaminant emissions data [6]. In this initiative the storage of relational data in a repository of searchable MatML documents was demonstrated. The use of MatML as a medium of data exchange across diverse storage formats was also depicted. This was with particular emphasis on data exchange over the Internet. Another important concept illustrated was the addition of value to the data through the eXensible Style Sheet Language (XSLT) to provide links to related aggregations of scientific information [6]. Consider the example of a relational database on volatile organic compounds (VOC). Figure 5 shows relationships between the tables in this database [6].

The application of MatML for storing data involved the following tasks. A mapping table was first created from an inner join of these database tables using their ID fields. Each record of the join had data on a particular contaminant. A mapping from the relational database to the MatML format was then developed with reference to the MatML schema [5]. This mapping associated the fields in the table to the elements in MatML. Fields with missing values, ID fields and fields useful only to database developers were not included in the mapping. A program was then written to generate a repository of MatML documents from a join of the database tables, following the rules in the mapping. Finally, the data in this repository was rendered for display on a browser by using an XSLT [28]. The XSLT had processing rules for adding value to the original data. Using this, the specifications were identified and hyperlinks were created to the concerned sources of data such as the NIST Chemistry WebBook [16].

The prime goal of this application was to promote standardization as required for consistency and reliability in storage, retrieval and analysis of the given data. It was realized through this effort that MatML was very useful for management and exchange of such materials property data on the web.

During the ASTM [4] Conference on Indoor Emissions Testing in Oct 2004, it was proposed that MatML be standardized to exchange contaminant emission data [6].

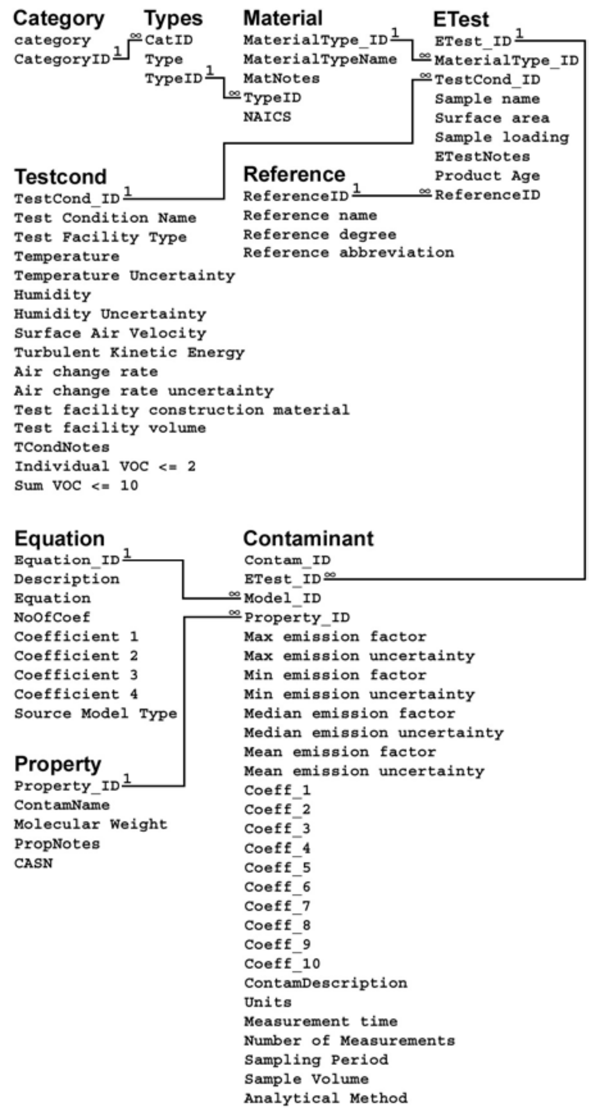

Figure 5: Relationships between Tables in the VOC (Volatile Organic Compounds) Database

3.3 Electronic Transfer of Data in Multiple Industries

Companies such as Boeing, Westmoreland Mechanical Testing & Research (WMTR) and Battelle consider the exchange of materials data as significant activities in their businesses. However, existing data exchange processes have been characterized as time consuming, labor intensive, error prone and expensive. Moreover, substantial data redundancy occurs, due to a variety of data structures and formats in use [20].

The use of MatML allowed these organizations to streamline and optimize the exchange and repurposing of materials property data. Using MatML also enabled significant cost efficiency, automation, and error reduction.

A MatML Data Exchange Project [20] was executed by WMTR, Battelle, and Boeing. The project involved using software systems from Granta Design and MSC Software, with project management provided by ASM International. The electronic data transfer project is detailed in Figure 6, which also shows the key stages enabled by MatML.

The effectiveness of MatML as the neutral medium for data exchange was borne out by the participants' successful use of MatML-encoded data in each of their own systems and processes.

An efficient data flow was enabled, which provided the input for statistical analysis of bulk data into design allowables for the MMPDS (Metallic Materials Properties Development and Standardization) used by the aerospace industry, which could also be extended, in principle, to other applications [20].

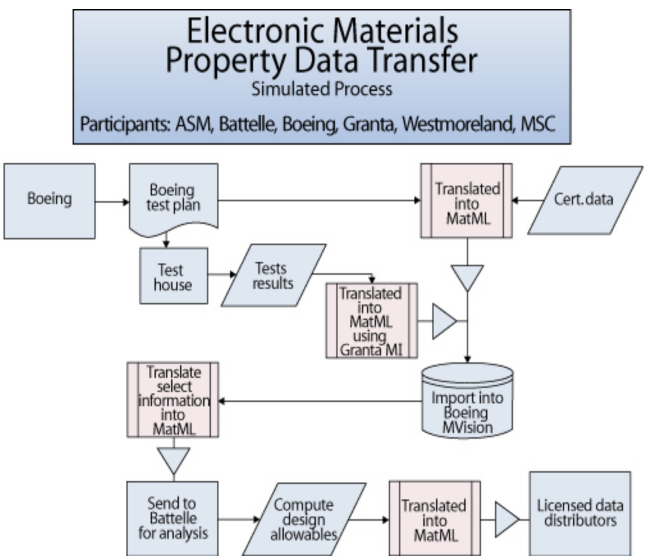

Figure 6: Electronic Transfer of Data in the MatML Data Exchange Project

4. DATA MINING APPLICATIONS

4.1 Statistical Process Control

The creation of design allowables in the MatML Data Exchange project sets the stage for applications such as control of processes based on statistical analysis. When the data among various organizations is easily exchanged in a common format, this permits the concerned parties to discuss the impact of processes in different industries and make decisions to control them. Moreover, the usable design allowables enable the documentation of information facilitating statistical analysis. Data mining techniques can be applied for learning [10]. For example, clustering is useful to group similar processes based on their results and classification is useful to analyze the causes of similarity between groups based on their input conditions [25]. Inferences drawn from such analysis analogous to a domain expert can be useful in decision-making to control similar processes in the future. Figure 7 shows an example of the grouping and reasoning strategies of domain experts (ref: CHTE [22]). These learning strategies can be automated to control new processes by analyzing existing ones [25].

In the literature, such analysis by integrating the data mining techniques of clustering and classification has been used in computational estimation [25]. It can also be used for process control. Storing the necessary information in MatML enhances such analysis by providing all the data in one place, though coming from different sources and in various formats including numbers, plain text and images. Thus MatML has an interesting application envisaged here.

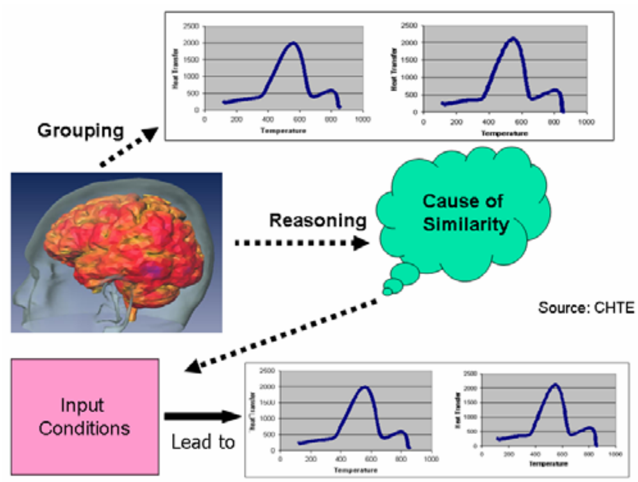

Figure 7: Learning analogous to Domain Experts for Process Control Applications

4.2 Failure Analysis

Data stored using MatML in various examples such as Building Processes Contaminant Emissions Data from NIST [16] and Military Mi17 Data [23] from the Department of Defense is useful to analyze failures. Data mining techniques such as association rule mining [19] could be applied here. In the literature, such rules have been used to predicting distortion tendencies, residual stress and other failure-related parameters in materials science processes [26]. These help analyze the causes of failure such as reasons for distortion in a part. The causes once detected help in designing process parameters so as to avoid similar problems in the future [26]. Figure 8 shows the potential steps involved in failure analysis with MatML by using association rules. Data from relational sources as well as raw data in other places is first converted to a common MatML format. This MatML data is then used for deriving association rules using the Apriori algorithm [19]. Interestingness measures are applied as per the knowledge of the domain to prune the rules. The rules that are not interesting are discarded. The interesting rules are useful for the purpose of failure analysis.

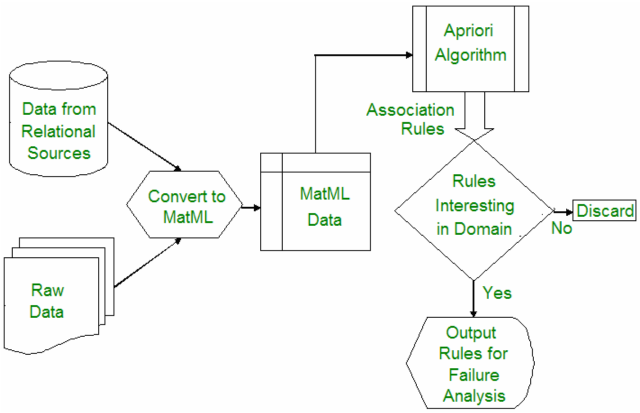

Figure 8: Steps in Failure Analysis with MatML

Other data mining techniques that could potentially be used to identify failures are outlier detection [10]. Once a normal pattern of behavior has been determined from existing data, a deviation from, normalcy could be useful in signaling potential failure. This could thereby help in failure prevention in advance.

Thus, the integration of data in a common repository using MatML aids analysis using data mining techniques such as association rules [19] and outlier detection [10]. The knowledge discovered from such analysis is useful in failure analysis in the corresponding industry.

4.3 Decision Support Systems

MatML finds interesting applications in decision support systems in targeted domains. An example of this is the QuenchMiner™ decision support system in the Heat Treating of Materials [27]. QuenchMiner™ is based on association analysis over experimental data pertaining to a rapid cooling process called *quenching*. This data involves input conditions such as agitation of a cooling medium during quenching of a material and the related observations such as cooling rates. The data is stored in databases and used for analysis by QuenchMiner™ [27].

However certain facts such as desired part suspension are not recorded in databases. Instead, details of experiments are found in the related literature. An interesting problem therefore is to extend rule-derivation to reference sources such as research papers. An interesting way to approach this problem is to first convert all the data into a common XML format and then extract rules. MatML provides some of the structure required for this conversion. In addition, a Heat Treating extension has been proposed to MatML and is being considered for standardization [24]. Automation of rule derivation from reference sources can hence be done by converting the reference data into XML using the MatML tagset along with the proposed extension. This research involves interesting issues such as capturing domain semantics during conversion and applying machine learning algorithms [15] in deriving rules after conversion.

Figure 9 shows an example of where MatML can fit into the architecture of such decision support systems. MatML can provide integrated data storage to mine over quenching experimental data and the related reference data for decision support in the QuenchMiner™ system [27]. Storing the data in this manner also enhances data visualization in presenting information to the users through the web.

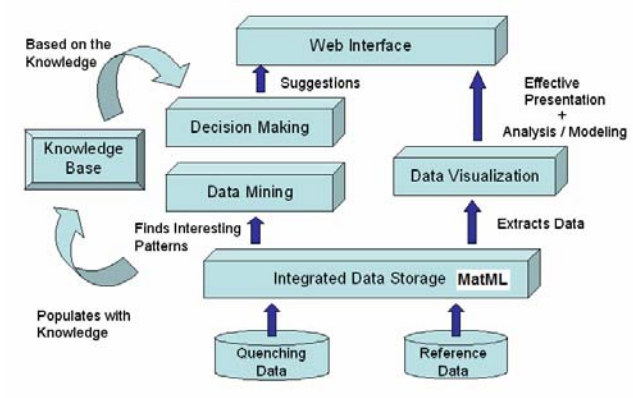

Figure 9: MatML for Data Mining and Visualization in Decision Support Systems

5. CHALLENGES AND ONGOING ISSUES

5.1 Varying Terminology

A significant challenge in promoting MatML is bridging the gap across domains using different terminology for concepts. This is being addressed through the development of a thesaurus or ontology to serve a broad array of materials science-related constituencies, which include electrical engineering and nanotechnology. Dealing with different units and data formats across domains and countries also presents an important challenge. This is being addressed through proposed automations of format conversions in addition to inclusion of glossary elements in the schema. The ontology development could involve the use of semantic web standards RDF and OWL [7].

5.2 Interfacing with other Markup Languages

Domain-specific markup languages are developed in different standards such as RelaxNG. Since MatML was developed in the W3C XML standard, interfacing with other markups poses interesting issues. This would possibly be addressed through ontological developments and extensions of the MatML schema as needed [24]. For example, such an extension was proposed at WPI, to capture the semantics of the heat treating of materials [24]. This is being considered by the MatML committee for standardization.

5.3 Guidance in Application-Specific use of MatML

The issue of guidance in using MatML elements is also a challenge, especially in the context of specific applications. We need to consider the fact that other data models and file formats were traditionally used for storage. This is being addressed through the development of user-friendly editors, some of which are application-specific, in addition to state-of-the-art conversion tools. Moreover, domain-specific examples [23] are being created with real data to illustrate the use of MatML in the context of specific applications. One such example is on MatML for storing and exchanging Mil7 data [23]. This clarifies the use of MatML tags for storing Military data by using real information. It also identifies areas where possible changes may be needed to make MatML even more user-friendly in the context of specific applications. NIST is very close to releasing a user-friendly

MatML editor [14, 16]. This would include polished user as well as technical documentation. The plan is to release the editor sometime in the next two months. Creating examples to illustrate data extraction from MatML using XQuery [7] is also a potential issue. Likewise, more issues are likely to be identified and addressed to promote further use of the Materials Markup Language, MatML.

6. CONCLUSIONS

MatML, the Materials Markup Language serves as the XML for storage and exchange of materials property data. It has a simple, understandable, flexible, extensible and cost-effective structure. It serves as a medium of communication among materials scientists worldwide and helps to connect related industries such as automobile, military, aerospace and manufacturing. Success stories with MatML include the development of materials digital libraries, management of building processes data and electronic data transfer in the MatML data exchange project. Data mining applications envisaged for MatML include statistical process control, failure analysis and decision support systems. MatML is being further enhanced with ontological developments, automated format conversions, comparison with related markups, schema extensions and user-friendly interfaces for guidance in specific applications.

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