DESCRIBING NANOMATERIALS: MEETING THE NEEDS OF DIVERSE DATA COMMUNITIES

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ABSTRACT

Fundamental in building any materials database is the capability to describe the materials whose data are contained therein accurately. While many systems exist for describing traditional materials, such as metals, polymers, ceramics, and others, the evolving field of nanotechnology presents new challenges. In this paper, we define the goals of a materials description system and the information categories used to describe traditional materials. We then discuss the challenges presented by materials on the nanoscale and suggest ways of overcoming those challenges.

Keywords: Materials databases, Materials description systems, Nanomaterials, Nanotechnology standards

1 INTRODUCTION

A fundamental and necessary condition for building materials databases, in general, is the existence of an accepted method for describing the materials contained therein. For "traditional" engineering materials and chemicals, multiple systems based on composition, chemistry, structure, specifications, and other criteria are available. For materials on the nanoscale (nanoscale is defined by ISO Technical Committee 229 (TC229) on Nanotechnology as approximately 1 nm to 100 nm) (International Organization for Standardization, 2010), which we call "nanomaterials" for convenience, an adequate description does not yet exist, even for use within a single discipline. The very fact that nanomaterials are of interest to multiple disciplines further complicates the problem.

Over the last few years, standard development organizations such as ISO TC229 have been trying to develop a nanomaterials description system, but progress has been slower than hoped. A robust and effective description system should take into account the needs and requirements of different disciplines, e.g., chemistry, physics, materials science, biology, medicine, toxicology, nutrition, environmental science, as well as the different requirements of diverse user communities: producers, researchers, regulators, legislators, consumers, and the general public. Among the challenges being addressed is the very nature of materials at the nanoscale. Particles of nanomaterials have properties dependent on surface characteristics different from "bulk" engineering materials and therefore require a more detailed description of surfaces. The number of atoms or molecules involved at dimensions from 1 nm to 1000s nm means that traditional chemical descriptions, including chemical bonding, are not adequate. Further, the properties of importance for different disciplines vary widely and in total represent a larger number of properties than those normally measured or required for more traditional materials.

Unfortunately, the normal pace of development for a description system by the R&D community is too slow for what is perceived as a potentially dangerous technological advancement by various segments of societies, including regulators, consumers, legislators, and the general populace. Even though the dangers of nanomaterials are not likely to be significantly different from dangers of existing materials, the scientific community cannot be passive and must actively work to develop a description system, based on scientific facts and commensurate with requirements and the time frame for action. Clearly such a system is essential for developers of nanomaterials databases.

In this paper, we will suggest some of the features necessary to create a robust system to describe materials on the nanoscale. The second section discusses the goals associated with any materials description system. The third section defines the major types of information needed for any materials description system. The fourth section discusses issues specific to the description of materials on the nanoscale. The paper concludes with a brief discussion of future work.

2 GOALS OF A MATERIALS DESCRIPTION SYSTEM

There are two primary goals for any system that provides a description of a material, regardless of the level of detail included, specifically *Uniqueness* and *Equivalency*.

By *Uniqueness*, we mean that the description is sufficient to differentiate the material being described from every other material. The uniqueness may apply simply to a material class: This material is a metal. It may be so specific as to apply to an individual piece of material: This material is Aluminum Alloy 6061 tube, manufactured according to BS (British Standard L118 T6 Tube hydraulically tested), and produced by Company XYZ. Uniqueness establishes which particular material or instance of a material is being described so that you know ***exactly what the material is***.

Equivalency, on the other hand, is the establishment of the fact that two materials or instances of a material are the same to some specified degree, such that their data sets can be combined into a larger data set. Equivalency allows you to know that ***two materials are the same***.

The goal of uniqueness is critical for a material description system as every use of materials data, from research to materials selection to product design to material purchase to regulations, depends on the description system's ability to be specific about the material involved. A well constructed materials description system allows for specifying uniqueness at several levels, from broad material class down to the description of an individual piece of material and intermediate levels in between. At each level, the system must carefully define the information content so there is no ambiguity.

The goal of equivalency serves many purposes. First, it recognizes that property data for most materials are generated over time by different testers for different purposes. The ability to gather all pertinent data together rests on a description system's capability to determine easily that the materials are the "same," at least to the degree of specificity desired. As a result, the traditional collections of materials data, whether in today's online databases or older printed handbooks, are useful because the aggregation of the data from different sources is scientifically correct. Equivalency also plays an important role in commerce and regulatory affairs. The data used to specify purchases again come from measurements often made on different batches of materials over time, and the combination of those data sets must be based on a description system's capability to determine equivalency. The same holds true for regulations of materials usage, for example, for aircraft design or toxicity testing, as we shall see later in the discussion of description systems for materials on the nanoscale.

3 THE INFORMATION CONTENT OF A MATERIALS DESCRIPTION SYSTEM

A wide variety of information is needed to describe any material fully, and that information can be categorized in a number of different ways. One convenient set of categories is shown in Figure 1, which is based upon work the authors have done in developing a number of materials data exchange standards (ASTM, 1993; International Organization for Standardization, 2008; www.matml.org). The specific items in each category differ depending on the type of material and the degree of detailed information desired. Examples are given below in Table 1.

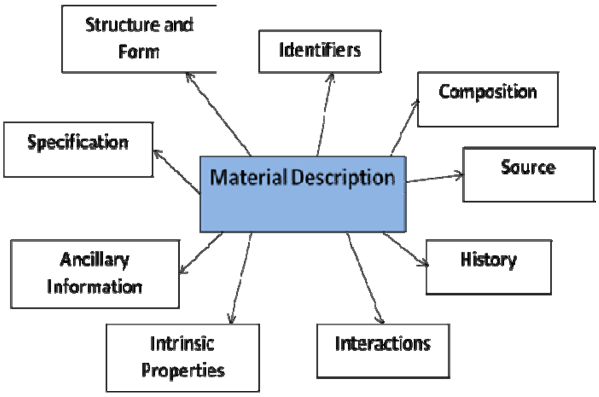

Figure 1. Information categories needed to describe a material

The information included in the categories of properties and interactions depends on the overall model of materials data being implemented. Two major approaches are used.

- Case 1: A material is described and the intrinsic properties included in the materials description are only those properties that the material was processed to have (See Figure 2)
- Case 2: All properties of a material are included in the materials description (In Figure 1, the category Intrinsic Properties is replace by Properties and now includes all properties, intrinsic and measured post-production)

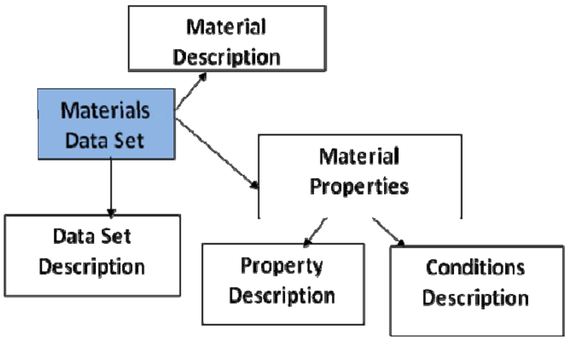

Figure 2. A Materials Data Set for Case 1. Materials properties, except for intrinsic properties, are not part of the materials description

In terms of implementation for data systems, the two approaches are similar, except for the amount of detail included in the materials description system as opposed to the description of a test method. In the first case, the properties and interactions, as well as the description of the test method used to determine those properties, which can require considerable detailed information, are not included in the materials description. As a practical matter, the development of standards for a materials description system or development of regulations about a particular material are much easier if the property and interaction information is not part of the description of the material itself.

Table 1. Information categories used in materials description systems

Information Category	*Types of Information Included*
Identifiers	Names: Formal, informal, commercial, synonyms
	Designations: Codes assigned by various groups
Specifications	Number and codes of specifications met by the material: Formal, informal, trade, government
Structure and Form	Spatial arrangements of components
	Size
	Shape
	External and internal geometry
	Surface geometry
	Size
Composition	Components and amounts
	Impurities
	Distribution
	Association among components (bonding, attachment, etc.)
	Aggregation
	Charge and charge distribution
Source	Who produced
	Where
	Why
	How (general)
History	Processing history
	Post-processing history
	How (detailed)
Intrinsic Properties	Those deliberately imparted to the material
	Those measured after production
	In-service experience
Interactions	Chemical
	Environmental
	In-service

4 MATERIALS DESCRIPTION ISSUES SPECIFIC TO MATERIALS ON THE NANOSCALE

As stated above, ISO TC229 (International Organization for Standardization, 2010) has defined a nanomaterial as a material with any external dimension in the nanoscale (approximately 1 to 100 nm) or having internal structure or surface structure in the nanoscale. In addition, the European Commission (Official Journal of the European Union, 2011) has recently defined nanomaterials as “A natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, having for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm - 100 nm.” Regardless of which definition is applied, the pertinent question is: *Does a description system for materials at the nanoscale require different categories of information from description systems for more traditional materials* (metals, alloys, ceramics, plastics, wood, etc.)? To begin to answer this question, let us look at *some* of the differences associated with materials on the nanoscale, as summarized below.

- Surface to volume ratio leading to changes from “bulk” properties (surface areas up to 1000 m^2 per gm)
- Different bulk and surface electronic structures
- Quantum size effects
- Dangling components on surface
- Chemical reactivity greatly different from more macroscopic forms (catalysis)
- New chemical forms (carbon nanotubes, titanium oxide, etc.)
- Small amount of impurities make big difference
- Self-assembly of ordered nanostructures
- Heterogeneous composition over the dimensions of the material

The consequences of these differences are summarized below.

- Chemical reactivity different and not predicable from bulk properties
- Quantum size effects result in unique properties vis-à-vis macroscopic materials
- Difficult to predict and control unique collective effects and self-assembly
- Poor knowledge of mechanisms of action
- Difficulty in building a unified model of nanomaterials
- Need for new nano-focused test methods
- Need to develop experience in actual use and performance

In addition to these differences and consequences, the number of scientific disciplines involved in the growing fields of nanotechnology and nanomaterials is quite large, especially compared to the use of tradition materials. The requirements for a description system for materials at the nanoscale must meet the needs of disciplines that include chemistry, materials science, physics, food science and technology, nutrition, medicine, toxicology, cellular and molecular biology, environmental science, and more.

5 FUTURE DIRECTIONS FOR DESCRIPTION SYSTEMS FOR MATERIALS ON THE NANOSCALE

Based on the considerations listed in Table I and other similar aspects, the development of a robust description of materials at the nanoscale faces many challenges that ISO TC 229 and other organizations are addressing. To help facilitate the development of a suitable description system, the International Council for Science (ICSU) (www.icsu.org) and CODATA (the ICSU Committee on Data for Science and Technology) (www.codata.org) sponsored a cross-disciplinary workshop in February 2012 to define and address some of the challenges on a multidisciplinary basis. Several of the challenges identified at the ICSU-CODATA Workshop are listed below in Table 2.

ISO TC229 working together with CODATA, ICSU, and materials organizations such as VAMAS (the Versailles Project on Advanced Materials and Standards) (www.vamas.org) plans to perform pre-normative work on addressing these challenges in a timely manner to develop the knowledge base for meaningful and accurate standards, including those for describing materials on the nanoscale. One of the most important conclusions of the workshop is that standards and regulations codify knowledge, and if knowledge is lacking, the standards and regulations are misleading and virtually useless. Given the great scientific, technical, and commercial potential of nanomaterials, the standardization process can and should drive the process of obtaining the needed knowledge.

Table 2. Some challenges hindering the development of a robust system for describing materials on the nanoscale

Challenge	Elaboration of the Challenge
Multiplicity of disciplines needing a description system	Chemistry, physics, materials science, food, nutrition, medicine, cellular and molecular biology, environmental science, many others
Multiplicity of uses	Materials testing, product design, materials selection, performance prediction, materials development, production engineering, product information systems, health and safety evaluation, legislation, regulations, standards
Lack of an unifying model of nanomaterials/particles	Development of a physical model(s) on materials at the nanoscale, taking into account the wide variety of such materials, from inorganic particles to carbon nanotubes to coated particles and more
Lack of proven test methods	Test methods that generate meaningful results for materials on the nanoscale are necessary before such information can be considered reliable
Lack of experience in correlating test results with service performance	For traditional materials, we have years of experience in correlating test results to performance in service
Poor knowledge of mechanisms of action	Greater understanding of the chemical, physical, physiological, and other mechanisms of actions are needed before we can establish which characteristics and properties are important

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