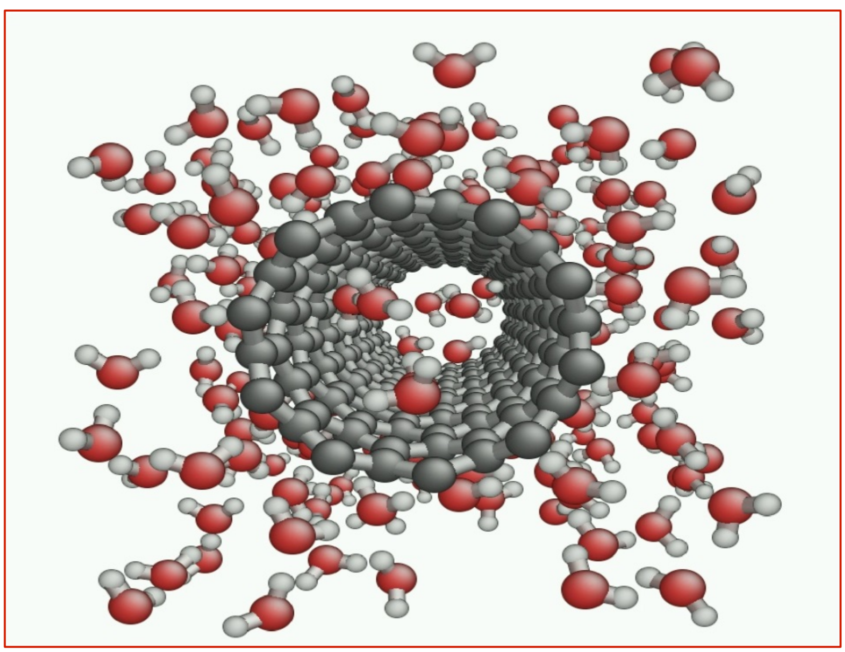
Uniform Description System for Materials on the Nanoscale

A Draft Framework

Developed by the CODATA/VAMAS Working Group on the Description of Nanomaterials



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1. Overview

A. Objective

A Uniform Description System (UDS) for materials on the nanoscale is being developed to meet the requirements of a broad range of scientific and technical disciplines and different user communities involved in nanomaterials. The **goal** is to define a complete set of information categories of descriptors that can be used by all communities interested in nanomaterials. This completeness does not imply that any one supplier of a nanomaterial description will likely use all the included information categories, subcategories, and descriptors. In fact, rarely will that happen. We hope, however, that as new information is developed, new information categories and descriptors will be defined and added into an evolving UDS.

The **purpose** of the UDS for materials on the nanoscale is twofold: Uniqueness and Equivalency. By *Uniqueness*, we mean the system has the ability within the broad range of disciplines and user communities to differentiate one nanomaterial from every other nanomaterial and to establish which particular nanomaterial or instance of a nanomaterial is being described. By *Equivalency*, we mean that the system can establish that two nanomaterials or nanomaterial instances are the same, as judged by different disciplines or user communities, in the sense that the set of descriptors adopted by the two or more communities are the same.

We recognize that new types and variations of nanomaterials are constantly being created and developed, and a robust system must also have the ability to evolve. The system cannot just be one of static measurement and classification. It must be capable of capturing the highly dynamic processes of evolutionary change that is characteristic of nanotechnology today.

B. Scope

The scope of this document is to provide a Framework for a Uniform Description System that describes materials on the nanoscale (as defined by, e.g., ISO/TC 229 and the European Commission – see below). This Framework is confined to describing a nanomaterial and does not address description of its performance. It can be used to describe:

Physical nanomaterials – nanomaterials made by any means for research, development, production, or other reasons

Virtual nanomaterials – nanomaterials that exist as models (usually computer-based) during the R&D stage of the material lifecycle

History – changes that take place to a nanomaterial throughout its processing and afterwards

C. Use

An effective and robust uniform description system for materials on the nanoscale should meet the needs and requirements of many user communities, including those outlined in Table 1 below. The Framework described in this document has been designed to address these needs, having been based in part on an extensive survey of diverse user communities. Most individual uses will have the need for specialized information peculiar to that need, but in aggregate, the present Framework should meet all those needs. As future needs are identified, the Framework can evolve to meet those needs.

Table 1. Uses of a Uniform Description System for Nanomaterials

Type of Use	Description of Use
Basic research	Development of new knowledge about nanomaterials without concern for their application
Applied research	Development of new knowledge about nanomaterials for specific applications
Synthesis and formulation	Describe and compare the structure, chemical components, and processing history of different nanomaterials
Evaluation of properties for applications	Reviewing existing nanomaterials for properties of interest to applications
Interactions with other materials	How nanomaterials might improve or degrade the properties or performance of another material/chemical/bio-substance
Commercial product design	Using a nanomaterial in an existing or future product sold to the public directly or indirectly
Materials selection	Choosing nanomaterials for an application
Materials performance prediction	Predicting the properties or performance of a nanomaterial itself or a material/substance containing a nanomaterial
New nanomaterials development	Development of new types or instances of nanomaterials
Materials development using nanomaterials with other materials	Development of new types or instances of materials/ substances that have nanomaterials as one component
Production engineering	Development of new or improved production of nanomaterials
Purchasing of nanomaterials	Specifying the purchase of nanomaterials
Purchasing of materials or substances containing nanomaterials	Specifying the purchase of materials/substances containing nanomaterials
Product and materials information systems	Building and disseminating information and data about nanomaterials or products containing nanomaterials
Environmental, health, and safety issues	Addressing issues related to concerns about environmental, health and safety issues related to nanomaterials
Legislation	Preparation of legislation dealing with nanomaterials or products containing nanomaterials
Regulations	Preparation of government or industry regulations dealing with nanomaterials or products containing nanomaterials
Standards	Preparation of standards dealing with nanomaterials or products containing nanomaterials
Reference materials	Materials used for test method evaluation and quality control of a specified nanomaterial property
Nanomaterials databases	Building and disseminating collections of data about nanomaterials, including data formats
Integration of different description approaches	Combining different systems used in specifications, nomenclature, and terminology
Data sharing	Formats for sharing information and data about nanomaterials
Knowledge discovery	Facilitating the discovery of new knowledge and understanding of

	nanomaterials through data science

2. Definitions

Descriptor

A descriptor (often called an attribute) is an item of information or data about an object (here a nanomaterial) that is measured, calculated, or assigned.

Information category

An information category is a group of descriptors that describe one aspect of a nanomaterial.

Note 1: An information category can be divided into one or more layers of subcategories for clarity or convenience in describing complex information.

Note 2: The responsibility for defining the descriptors in an information category or subcategory can be formally assumed by a standards development organization, a national or international regulatory authority, or other competent organization.

Nanomaterial

Several international definitions of a nanomaterial have been adopted. This Framework is intended to be used irrespective of the precise definition of the term nanomaterial. It should be able to describe materials that fit the nanomaterials definitions, as well as those materials with nanoscale features that maybe are just outside the range of materials considered nanomaterials according to a specific version of a specific definition. Nevertheless, two international definitions where considered more carefully than others, when writing this draft UDS:

The ISO/TC 229 definition[1] of a ***nanomaterial*** is as follows:

"A Nanomaterial is a material with any external dimension in the nanoscale [approximately 1 nm to 100 nm] and or having internal structure or surface structure in the nanoscale."

The European Commission definition[2] of a ***nanomaterial*** is as follows.

"A natural, incidental or manufactured material containing particles, in an unbound state or as an aggregate or as an agglomerate and where, 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.

"In specific cases and where warranted by concerns for the environment, health, safety or competitiveness the number size distribution threshold of 50 % may be replaced by a threshold between 1 and 50 %.

"By derogation from the above, fullerenes, graphene flakes and single wall carbon nanotubes with one or more external dimensions below 1 nm should be considered as nanomaterials."

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[1] ISO/TS 800004-1:2010(E)
[2] http://ec.europa.eu/environment/chemicals/nanotech/#definition

Nanomaterial instance

A specific piece of nanomaterial that physically exists.

3. Additional Background

The Framework is provided as a mechanism to identify systematically the universe of descriptors required to describe nanomaterials uniformly regardless of the discipline, application, or use involved. Previous efforts to develop description systems have focused on a limited number of information categories resulting in incomplete description systems. The approach presented here not only supports the development of a complete description system, but also enables integration of different approaches that produces partial description systems. Using a systematic framework allows the nanomaterials community to identify areas in which knowledge of what are the appropriate descriptors is lacking and to address those deficiencies.

4. General Outline

The Framework for the Uniform Description System comprises a set of four information categories, which are explained in more detail below (see Figure 1).

1) General identifiers
2) Characterization
3) Life cycle history
4) Specifications

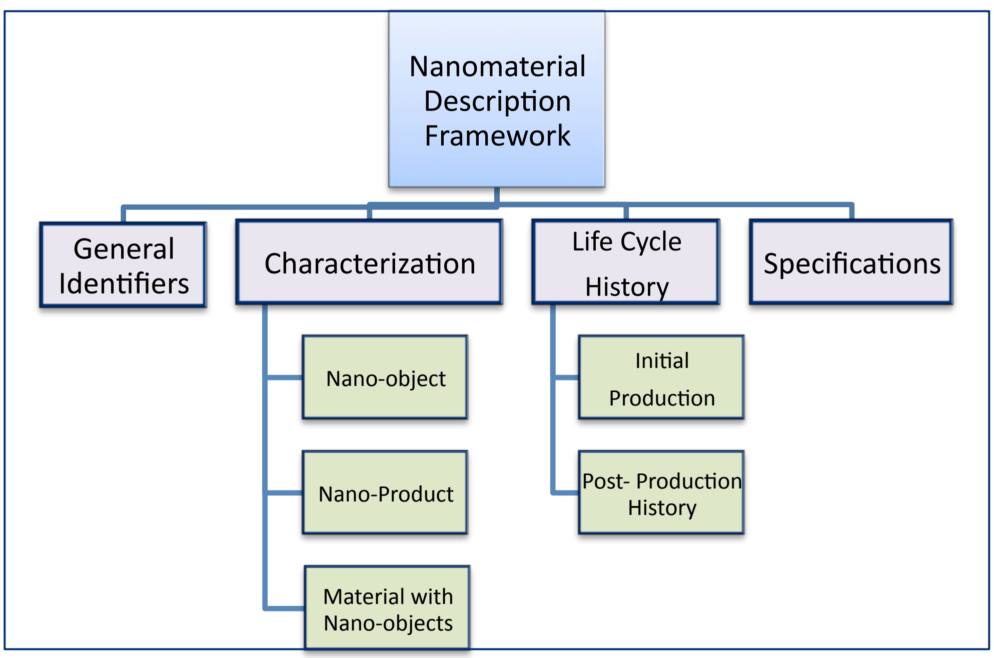

Figure 1. Schematic of the four main information categories and major subcategories of the Framework for a nanomaterial uniform description system.

Each of these information categories contains numerous subcategories that in turn contain the descriptors that provide the detailed information and data comprising a complete uniform description system. The system is not hierarchical except that subcategories refer back to the main categories. Different users of the description system will use different subcategories and descriptors to a lesser or greater extent. These categories and subcategories can be used to create an ontology for nanomaterials that can be used to support many different types of applications.

The Framework can also support the development of one or more technical dictionaries of descriptors or insertion of existing systems of subcategories and descriptors as developed by different organizations such as standards development organizations, international scientific and technical unions, and professional societies. Such organizations may take responsibility for maintaining and expanding subcategories or the descriptors contained therein based on the needs of their communities. The Framework also can be used as the basis for data models and ontologies used to build nanomaterials informatics systems.

1) General Identifiers

This category contains a set of general and specific information used to name and classify a nanomaterial. The four subcategories are

a) Common names
b) Formal names
c) Class
d) Identification numbers and codes

a) Common names

One or more names a nanomaterial is called. These names arise from many sources, but are not authoritative.

b) Formal name(s)

One or more names assigned to a nanomaterial by some authority; the name of the authority can be included as a descriptor.

c) Class

One or more class names to which a nanomaterial can be assigned; if the class is defined by an authority, information on the authority, such as a standards development organization, government agency, international scientific union, or internal company policy, should be included.

In this category, only the class name is given, e.g., single-wall carbon nanotube, and other details are specified in other categories. Examples of commonly used classes for nanomaterials include the following.

- Form, such as plate, rod, sphere, hollow plate, hollow rod, hollow sphere, textured, MCM-41
- Elemental, such as metals, nonmetals, metalloids, alkali metals, alkaline earths, transition metals, halogens, noble gases, rare earths, lanthanides, actinides
- Naturally occurring/manufactured
- Organic or inorganic

- Chemical type, such as covalent bonded, hydrogen bonded, ionic bonded, metal bonded, carbide, oxide, monomer, micelle, lipids, proteins, RNA-based, DNA –based, virus
- Crystalline Structure, such as triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal, cubic (simple, BCC, FCC),
- Structure, such as atom or molecule within another molecule, atoms or molecule attached to another, geometric structures built from DNA sections, polymer, dendrimer
- Application, such as catalysis, quantum dot, carrier for pharmaceutical, mechanical strength, electrical conductivity, optical index of refraction, magnetic moment

d) Identification numbers and codes

These are numbers and codes assigned to a nanomaterial by some authority; the name of the authority should be included. Identification numbers and codes do not necessarily contain embedded information and are usually reference numbers or codes to a document issued by an authority that contains additional information about the nanomaterial. An example of an identification code is a Chemical Abstracts Registry number.

An identification number or code is different from a specification number or code. An identification number or code references back to a definition of what something is; a specification number or code references back to a definition of how something was produced or to the criteria to which is was produced.

2) Characterization

Nanomaterials can be divided into three types based on the amount and the presence of other materials.

a) an individual nano-object;
b) a collection of nano-objects, which are called nano-products; and
c) a bulk material that has nano-objects as components.

Each type requires a different set of descriptors for description. Each of these instances will be described below.

a) Characterization of Individual Nano-objects

It is at the scale of individual nano-objects that the complexity and uniqueness of nanomaterials is most clearly demonstrated. The term nano-object is defined in ISO/TS 80004-1:2010, 3.5 as a material with one, two or three external dimensions in the nanoscale. The nanoscale dimensions involved, 1 nm to 100 nm, mean that the quantum effects that make nanomaterials so interesting come into full play.

The following eight subcategories, as shown in Figure 2, comprise the characterization of an individual nano-object. In the discussion that follows, the term “nano-object” refers to an individual nano-object.

1. Form and shape
2. Size
3. Chemical composition
4. Physical structure
5. Crystallographic structure
6. Surface description
7. Defining Properties
8. Stability

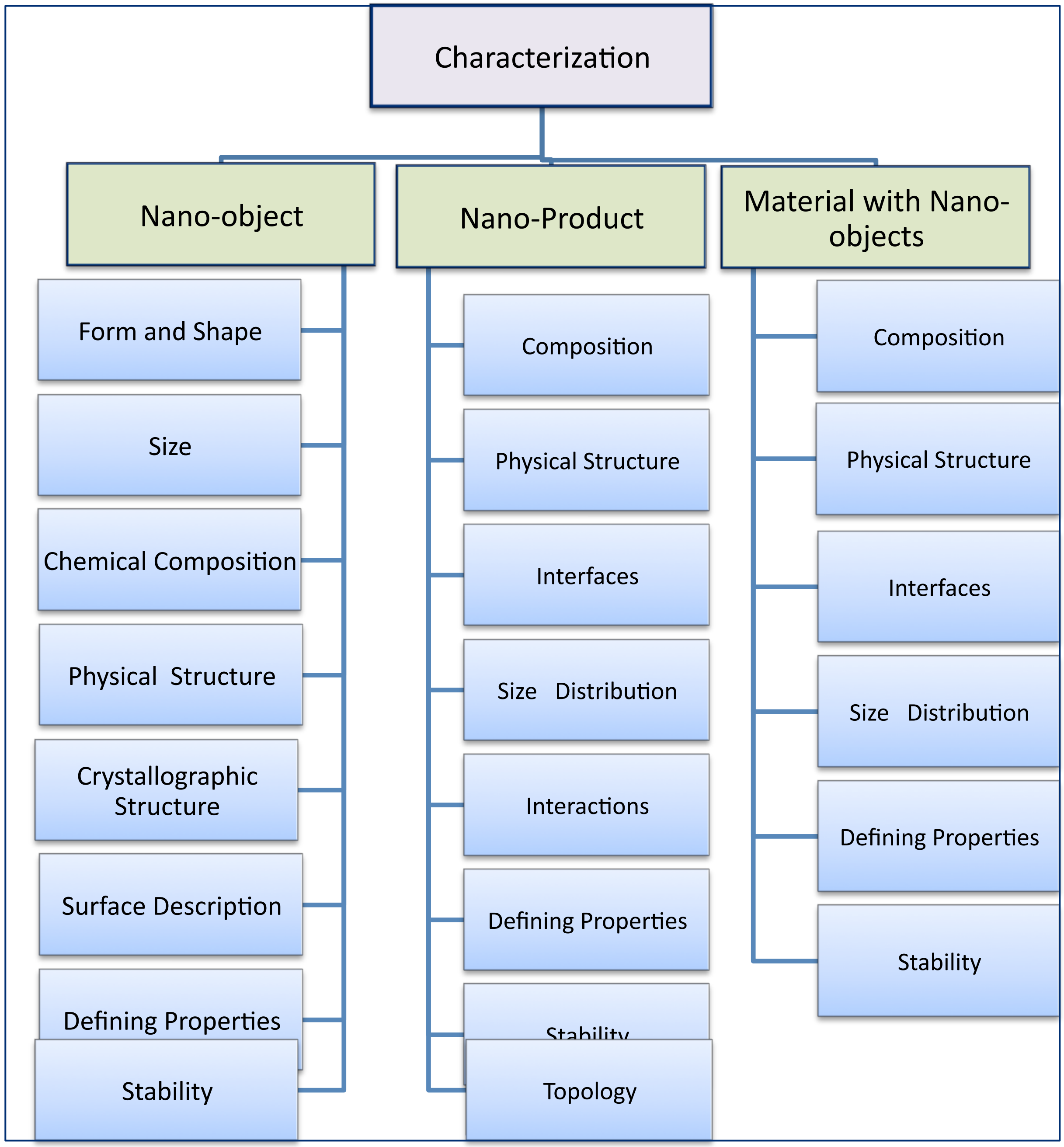

Figure 2. Schematic of the main information subcategories in the characterization of an individual nanomaterial.

1. Form and Shape

The characterization of the geometrical form and shape of a nano-object is critical as its properties and reactivity are strongly dependent on this factor. Considerable effort has gone into establishing standard definitions for many forms, and as new forms are discovered, addition definitions are developed. The most common criterion for defining a form is by their general three-dimensional geometry.

ISO/TC 229 has defined several common forms including: nanoparticle, nanorod, nanotube, nanoplate, nanostar, nanosheet, nanocone, and nanocage. It is anticipated that ISO/TC 229 will continue to standardize the terminology associated with the form and shape of newly discovered nano-objects.

2. Size

The dimensions needed to specify the size (internal and external dimensions) of different nano-objects forms vary according the form. In addition, some forms have ambiguity in their definition, e.g., at what ratio of diameter to length can a rod also be considered a particle; similarly for plates. In many instances, the smallest dimension (such as wall thickness) is often given in terms of the number of atomic or molecular layers.

In an ideal situation, each nano-object form would have a well-defined set of size measurements to be reported so that property-size correlations could be made. At present, no group has the responsibility for developing the relevant standard size measurements for different forms. ISO/TC 24/SC 4 (Particle characterization), however, is a strong candidate. They have a lot of standards on the size descriptors for different shaped objects as well as the size analysis standards.

3. Chemical Composition

The chemical composition of a nano-object can be expressed in several ways, e.g., in terms of the principal atoms or molecules present, or as a percentage of various components. When a nano-object has multiple internal structures, such as a core, shell, surface, or covering, the chemical composition for each structure may be given as needed.

The chemical composition comprises the list of chemical components (on an atomic or molecular basis), their amounts, and their chemical bonding (including structural formula), when appropriate.

The International Union of Pure and Applied Chemistry (IUPAC) is the major international authority for chemical nomenclature and is the appropriate body to try to extend current chemical nomenclature and bonding technology to nano-objects. At the same time, other disciplines, such as food science and paint pigment technology, have developed specialized terminology to describe the chemical composition of materials and need to examine if their system for describing chemical composition needs to be extended.

This subcategory includes chemical structural identifiers such as the IUPAC International Chemical Identifier (InChI) and those used by government and private company chemical databases and other chemical software. Chemical structural identifiers, by definition, contain embedded information from which all or part of the chemical structure of a nanomaterial can be deduced.

4. Physical Structure

Nano-objects can have internal structures depending on their complexity. Because nano-objects take so many different forms, shapes, and sizes, different physical structure models are possible. Many nano-objects are layered or have other inhomogeneities. These structural characteristics need to be described in detail in terms of the composition of each component, its place in the overall structure, and other details, e.g., the structural features of a multi-layered nanotube. Some nano-objects are synthesized to have specific pore sizes, e.g., MCM-41, for catalytic purposes. The description of structural defects and impurities, whether intentional or unintentional, needs to include details of the amount, identity, and location of each defect/impurity.

Some classes of nano-objects, such as carbon nanotubes, have had their physical structure considered in detailed; others have not. At present, no system exists for describing the physical structure of nano-objects, or for physical models that could be used.

5. Crystallographic Structure

The crystallographic structure of nano-objects is very important. The International Union of Crystallographers (IUCr) has developed a comprehensive system for describing the details of crystallographic structure that can be used and extended for nano-objects.

6. Surface Description

Structured surfaces on the nanoscale are increasingly being produced to have unique and useful electronic and photonic properties. Because of the reactivity of one or more surfaces in a nano-object, a nano-object will have adherents on their surface, especially when a nano-object is in a biological or environmental fluid. These surface structures may also manifest themselves as an altered external shape. The description of the surface structure of a nano-object is important. That description needs to include surface charge and surface attachments.

No system for describing the surface characteristics of nano-objects now exists, though ISO/TC 201 is trying to.

7. Defining Properties

Defining properties are the properties of a nano-object that (1) can be calculated from first principles, such as elastic constants or density; (2) are test-independent, such as melting point, thermal conductivity, etc.; or (3) have been deliberately imparted to a material to meet a specification, such as producing a nano material with a specific chirality.

Very often a nano-object is produced to have specific properties, for example to meet the requirements of an internal or external specification, to have some commercial advantage, or to determine how a particular material might perform in service. The set of properties that have been deliberately imparted to a nano-object are part of the defining properties and are considered part of the nanomaterial description.

These properties are differentiated from those properties that are measured not in the course of a nano-object production but afterwards in tests unrelated to the production process. Typical properties of this type include the following.

- Color
- Dispersability
- Optical properties, e.g. refractive index
- Solubility in water or other liquids

This framework allows specification of a list of defining properties. It is anticipated that different disciplines and user communities will have different sets of defining properties critical for describing nano-objects in their context.

8. Stability

The stability of a nano-object is an important characteristic and as nanomaterials in general are quite reactive, characterizing stability is useful information. To date no standard way of describing nano-object stability exists. Inspiration may be found in the ISO Guides 34 and 35 documenting the approaches to be followed by reference material producers to assess the stability of (the certified properties of) reference materials.

b) Characterization of Nano-Products

Aside from the assemblage of a single nano-object from individual atoms, multiple nano-objects are usually produced at one time. In addition, different nano-objects may be combined together for better properties. These larger amounts of nanomaterials are called nano-products and are composed solely of nano-objects and possible impurities. At present, very little work has been done to produce a systematic approach to describing nano-products. The following subcategories comprise the characterization of a nano-product. Many of these subcategories are the same as those used to describe an individual nano-object.

1. Composition
2. Physical Structure
3. Interfaces
4. Size Distribution
5. Interactions
6. Defining properties
7. Stability
8. Topology

1. Composition

The components of a nano-product are individual nano-objects, adherents, and impurities. The nano-objects are described using the information categories applicable to them as defined above. By composition, we mean the amount of each component. As with other materials, the amount can be expressed as weight or molecular percent.

2. Physical Structure

The physical structure of a nano-product is usually described by a physical model. Examples of the details that need to be specified include: the location of components; homogeneity or lack thereof; internal and surface structure; macromolecular nature (e.g., polymer, dendrimer); or type of aggregation or agglomeration. The arrangement of the components within a nano-product can be complex. For example, polymeric nano-objects can be arranged in many ways.

At present no system for describing the physical structure of a nano-product exists.

3. Interfaces

Molecular functionalization of the surface of a nano-object can be weakly or tightly bound. The interfaces among two or more nano-objects found within a nano-product are very important and can be quite complex. One example is the interactions of a collection of atoms inside a C_{60} or C_{80} nano-object. Individual nano-objects can also associate both weakly (forming agglomerates) or strongly (forming aggregates).

Very little work has been done on describing interfaces among nano-objects within nano-products.

4. Size Distribution

When nanomaterials are produced, a range of sizes are made. The size distribution is important information to describe, and the details for describing the distribution must be well defined. At present no specific guidelines exist for reliable assessment of size distributions in the nanoscale, though many techniques are being developed to measure size distribution.[3]

[3] Requirements on measurements for the implementation of the European Commission definition of the term "nanomaterials," T. Linsinger, et al, JRC Reference Report EUR 25404 EN

5. Interactions

Some interactions can be described under interfaces above. Other interactions could also describe the types of bonding between nano-objects - electrostatic, ionic, and covalent bonding between atoms of the interacting nano-objects. This includes the more complex many-body effects among all the atoms of the interacting nano-objects, e.g., plasmonic phenomena; photonic phenomena. At present no work is ongoing with respect to this descriptor.

6. Defining Properties

Defining properties are the properties of a nano-product have the same characteristics as for nano-objects, as defined above.

7. Stability

The stability of nano-product is an important characteristic and as nanomaterials in general are quite reactive, characterizing stability is useful information. Stability concerns can be important in both simple cases of the storage of nano-products and complex situation of the stability of a nano-product in service.

To date no standard way of specifically describing nanomaterial stability exists.

8. Topology

Topology is the description of the overall geometry of a nano-product and its components (where each component can be one or more nano-objects) including the relative position in space of the components, e.g., totally or partially internal or external to each other, and their connectedness and boundaries, done in such a way that a correlation between the shape and the properties of a nano-product can be ascertained. At present there is no system under development to describe systematically the topological features of a nano-product.

c) Characterization of Materials Containing Nano-objects

Commercial uses of nanomaterials often involve existing materials that incorporate nanomaterials to enhance one or more properties or functionalities. As more complex materials containing nano-objects are made, the description of their characteristics becomes more complicated. This is especially true for biomaterials and structural materials.

The description of materials containing nano-objects begins with the description of the nano-objects themselves plus a conventional description of the bulk or filler material. At present, however, very little work has been done to produce a systematic approach to describing materials containing nano-objects. The following subcategories comprise the characterization of a material containing nano-objects.

1. Composition
2. Physical Structure
3. Interfaces
4. Size Distribution
5. Defining properties
6. Stability
7. Topology

1. Composition

The components of these materials are individual nano-objects, nano-products, adherents, impurities and the bulk or filler material. The nano-objects are described using the information subcategories and descriptors applicable to them. This information for nano-objects must be combined with information about the bulk and filler material. By composition, we mean the amount of the nano-objects, adherents, and impurities, as well as similar information about the bulk and filler material. As with other materials, the amount can be expressed as weight or molecular percent.

2. Physical Structure

The basic structure of a material containing nano-objects is normally very complicated. The physical modes of physical structure are generally empirical and material specific. Examples of the details that need to be specified include: number of components; homogeneity or lack thereof; internal and surface structure; macromolecular nature (e.g., polymer, dendrimer); or type of aggregation or agglomeration. The arrangement of the components within a these materials can be complex.

At present there is no systematic approach to developing the description of the physical structure of materials containing nano-objects. Whether a systematic approach is possible needs to be determined.

3. Interfaces

The interfaces among nano-objects and bulk and filler materials are critical in determining the properties and performance of materials containing nano-objects. In addition to simple considerations such as the type of "bonding" among the various components, correlation of the type and strength of these interfaces are important in understanding differences between predicted and actual performance.

Simple materials now under research and commercial development often have the interfaces closely studied, but no general system for classifying and describing such interfaces exists. Clearly, as more materials containing nano-objects enter into production and commerce, this subcategory will need additional attention.

4. Size Distribution

When nano-objects are embedded into bulk materials, the nano-objects often come in a variety of sizes. The size distribution of the nano-objects is important information to describe, and the details for describing the distribution must to be well defined. At present no guidelines exist for measuring size distributions of nano-objects inside more or less complex matrices. As mentioned in the discussion of size distribution under nano-products, many techniques are being developed to measure size distribution.

5. Defining Properties

Defining properties are the properties of a material containing nano-objects have the same characteristics as for nano-objects, as defined previously.

6. Stability

The stability of materials containing nano-objects is an important characteristic and as nanomaterials in general are quite reactive, characterizing stability is useful information. To date no standard way of describing nanomaterial stability exists.

3) Life Cycle History

The lifecycle of a nanomaterial is assumed to have a distinct initial production phase followed by one or more post-production phases. The post-production phase may simply be storage after initial production or a more complex transformation.

Much effort is being made by several engineering communities to develop process models that are applicable to a wide variety of processes. As a Uniform Description system for nanomaterials progresses, these models need to be reviewed and utilized to the extent possible.

An initial discussion of the initial production phase and a generic post-production phase are given below.

A. Initial Production

The initial production information category contains the information relevant to how a nanomaterial was initially synthesized, formulated, produced or manufactured to achieve its primary structure and properties. The production of a nanomaterial in the context of a research or experimental environment is quite different from production in a commercial setting. The amount and type of processing history information reported will vary greatly depending on the circumstances as well as the source of the information. Many companies share very few processing details, relying instead on highlighting "unique" properties of their materials. Publicly funded research papers, however, might contain extreme detail when authored by conscientious researchers.

The general subcategories here are as follows.

1. Source
2. Production Details
3. Production Documentation

1. Source

Source contains the information of where, when, and by whom a material was produced. Source also can contain information on why the material was produced and potential uses of a material. The type and amount of information included depend on who is compiling the information and for what purpose.

Details about the source include the following: producer name, producer location, producer contact information

2. Production Detail

The production details describe all the details of the initial production, including: production date, processing procedures, lot numbers, etc.

3. Production Documentation

The production documentation describes the type of documentation that exists, the production reason, potential uses, etc.

B. Post Production History

In this subcategory, information of how a nanomaterial was storage, processed, used, or transformed would be included. Information on exposure history provides a means to record the conditions to which a nanomaterial has been exposed subsequent to its being put produced or being put into service. Because nanomaterials can be very reactive, this information is needed to establish that the nanomaterial continues to meet new or revised design criteria.

The general subcategories here are as follows.

1. Post-Production Agent

2. Post-Production Details
3. Post-Production Documentation

1. Post-Production Agent

The agent is the person or organization who stored, processed, or transformed a nanomaterial after it was initially produced.

2. Post-Production Detail

The production details describe all the details of the initial production, including: production date, processing procedures, lot numbers, etc.

3. Post-Production Documentation

The production documentation describes the type of documentation that exists, the production reason, potential uses, etc.

4) Specifications

This category contains detailed information about specification documentation according to which a nanomaterial has been produced or documented. Examples of typical subcategories related to specifications are as follows.

1. Name – the name given in the specification document
2. Specification title – title of specification document
3. Specification authority – authority issuing specification document
4. Date of issue – date of issue for specification document
5. Type of specification – type of specification document [standard specification, regulation, company specification, purchase order, material list, etc.]
6. Version of specification – version of the specification document
7. Identification number – when the number refers back to a document or reference source that specifies the nanomaterial

This subcategory can also contain information about the registration of a nanomaterial in a government, public or private registration system, including the authority controlling the registration system. The fact that a nanomaterial is registered in such a system does not mean that it has specific properties or interactions; that information can only be determined by referring back to the registration system itself.

4. Activity to develop the Description System - Next Steps

The Framework presented above is a **work in progress**, though hopefully complete in one sense: The four broad information categories provide the large groupings under which most if not all descriptors commonly or less-commonly used to describe nanomaterials can be placed systematically. The next step is to review and refine the major subcategories under each category. Then, to the extent possible, further subcategories or descriptors themselves need to be defined and added to the Framework. By this means the Uniform Description System will evolve.

As mentioned through the discussion of the various information categories, some groups are already working at defining the subcategories and descriptors more completely. As shown in Table 2 below, however, many key categories and subcategories are not being worked upon. For the uniform description system to become a reality, this has to change.

Table 2. Status of Work on Various Categories and Subcategories for Describing Nanomaterials	
Information Category	**Group Presently Working on the Category**
General Identifiers	
Common Names	
Specific Names	Many groups
Classes	Many groups
Identification codes	Many groups
Characterization	
Nano-object	
Form and shape	ISO/TC 229
Size	ISO/TC 24/SC 4, See also JRC paper (Reference 3)
Chemical composition	IUPAC
Physical structure	
Crystallographic structure	IUCr
Surface description	ISO/TC 201
Defining properties	
Stability	
Nano-product	
Composition	
Interfaces	
Interactions	
Size distribution	ISO/TC 24/SC 4, ISO/TC 229, VAMAS, See also JRC paper (Reference 3)
Defining properties	
Stability	
Topology	
Materials with nano-objects	
Composition	
Interfaces	
Size distribution	CEN/TC 352, See also JRC paper (Reference 3)
Defining properties	
Stability	
Life cycle history	Use process description models
Initial production	
Source	
Production details	
Production documentation	
Post-production history	
Post-production agent	
Post-production details	

Post-production documentation	
Specifications	

5. Different Disciplines

The Framework described above is intended to cover a broad range of nanomaterials and is applicable for most uses and disciplines. Different application areas, however, may have additional specialized requirements that reflect the peculiarities of different situation in which nanomaterials must be described accurately.

The intent of the CODATA/VAMAS Working Group is to bring together as many different nanomaterials communities so they can use the Framework as the base description system and add additional categories and descriptors as needed. We hope different disciplines review the Framework carefully from several viewpoints.

- Does the Framework cover the information used to describe nanomaterials in your discipline?
- Are there subcategories of information for which your discipline naturally would define detailed descriptors? If so, is there ongoing work to define descriptors?
- Are there additional uses for a Uniform Description System besides those listed in Table 1?

6. The Future

The Framework presented here is the second step in a series of steps that started with identifying requirements. Work will hopefully continue not only on a consensus-driven Framework for the UDS, but also with commitments from organizations to develop the detailed descriptors under each subcategory needed to make the UDS usable and useful.

This Framework can be circulated freely and comments, suggestions, improvements, and criticisms can be sent to the compilers at udsnano@udsnano.org

Once comments are received, the Framework will be updated and used as the basis for a series of three international, regionally located (Europe, Asia, and North America) conferences to be held in 2014. These meetings will focus on three areas of interest.

1. Extending, improving, and implementing the Framework and moving all or portions of it from a pre-standardization effort into the standards arena as appropriate.
2. Highlighting how the Framework will be used by different disciplines and applications areas to advance the development and use of nanomaterials.
3. How the Framework can be sued as a foundation for nanoinformatics, leading to new data collections, data tools, and software to exploit the growing body of knowledge about nanomaterials.

The 3 October 2013 version of the Framework for a Uniform Description of Nanomaterials has been prepared by the following people under the auspices the CODATA-VAMAS Working Group on the Description of Nanomaterials.

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