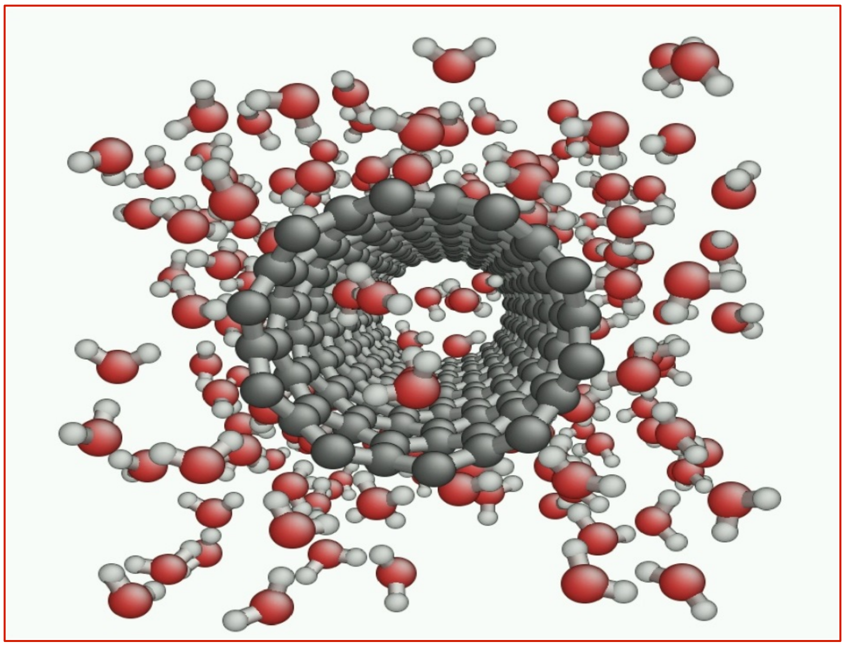
# Uniform Description System for Materials on the Nanoscale

## Prepared by the CODATA-VAMAS Working Group on the Description of Nanomaterials



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# I. Overall Introduction

Following is a draft of the Uniform Description System for Materials on the Nanoscale (UDS) as prepared by the CODATA-VAMAS Working Group (WG) on the Description of Nanomaterials. This draft is based on a Framework for the UDS as previously developed by the CODATA-VAMAS WG [1].

Following discovery by experimentation or design, the process of using a new material goes through stages. First it becomes the focus of research and development (R&D) with the intent of understanding how it behaves and then demonstrating such understanding through control of various parameters to give predictable behavior. During this discovery process, the need to accurately describe the material grows. Finally there comes the time when it is necessary to describe the material to a much larger group of people.

The above process has been followed during the past 20 years of growing interest in nanomaterials, a group of novel materials that offer great promise for vastly improved properties and functionalities caused by nanoscale features. As the first wave of nanomaterials are being incorporated into products and new nanomaterials continually being developed, they have become of great interest to a wide diversity of stakeholders ranging from researchers to product manufacturers to health and environmental experts to regulators and legislatures to consumer and the general public. All new materials offer both the promise of benefits and the potential of risks; nanomaterials are no different.

What is clear about nanomaterials is that the combination of small scale, exotic behaviors, and significant commercial value brings an interesting challenge: How do we know exactly which nanomaterial as well as which of its features are important? Nanomaterials are larger than ordinary inorganic, organic, and biochemical molecules with significantly more features that provide a wide variety of functionalities. At the same time, the description methods for "bulk" materials are insufficient to describe the nanoscale features such as form, quantum effects, and surface properties that make nanomaterials interesting. Further nanomaterials are of great interest to a wide group of scientific disciplines, product developers, and user communities, all of which need to communicate effectively with one another.

To restate the challenge: How can one describe a nanomaterial accurately on a multi-discipline, multi-user basis recognizing that the science and technology of nanomaterials continues to evolve? The following attempts to answer that question.

# II. Definitions

Several terms are used through this document and are defined as follows.

***Descriptor***: Numerical data or text that expresses the measurement, observation or calculational result of some aspect on an object

Note 1: A descriptor conveys both the semantics of the results as well as the result itself. A general model of a descriptor is given in Appendix A.

***Information category***: a set or group of related descriptors that represent a property, characteristic, or feature of an object

Note 1: Information categories may be hierarchical and contain subcategories (referred to as such) each containing a set of descriptors.

Note 2: Information categories, and their subcategories, are constructed to convey understanding of the structure, properties, features, and performance of an object.

Note 3: A descriptor may occur in more than one information category. It is the responsibility of the owner of data or information resources using an information category to ensure that data and information redundancy is adequately addressed.

***Nano-object***: An individual material item with at least one dimension on the nanoscale (about 1 to 100 nanometers) that has distinct boundaries in all dimensions and cannot be further subdivided without losing functionality

***Ensemble of nano-objects***: a group of nano-objects that functions as a unit is some prescribed manner.

Note 1: An ensemble can be made of identical or different nano-objects

Note 2. The grouping of nano-objects within an ensemble can occur through a variety of forces (direct chemical bonding, van der Waals attraction, electrostatic interactions, third party mediation, i.e. a catalyst)

***Bulk material***: A material that has all external physical dimensions larger than the nanoscale

Note 1: A bulk material may have internal and surface features discernable on the nanoscale.

***Uniqueness:*** The ability of a description system to differentiate one object (here a nanomaterial) from every other object (all other nanomaterials) and to establish which particular object (nanomaterial) is being described within the broad range of disciplines and user communities

**Equivalency:** The ability of a description system to establish that two objects (nanomaterials), as assessed by different disciplines or user communities, are the same to whatever degree desired.

# III. Background

The approach taken herein has been to identify the broad types of information that are used through the nanomaterials community to describe a nanomaterial as completely as possible. The goal has been to establish the uniqueness of a nanomaterial so it is clear which nanomaterial is being described and to allow the establishment of the equivalency of two nanomaterials to whatever level desired. The terms *equivalency* and *uniqueness* are described in the definitions.

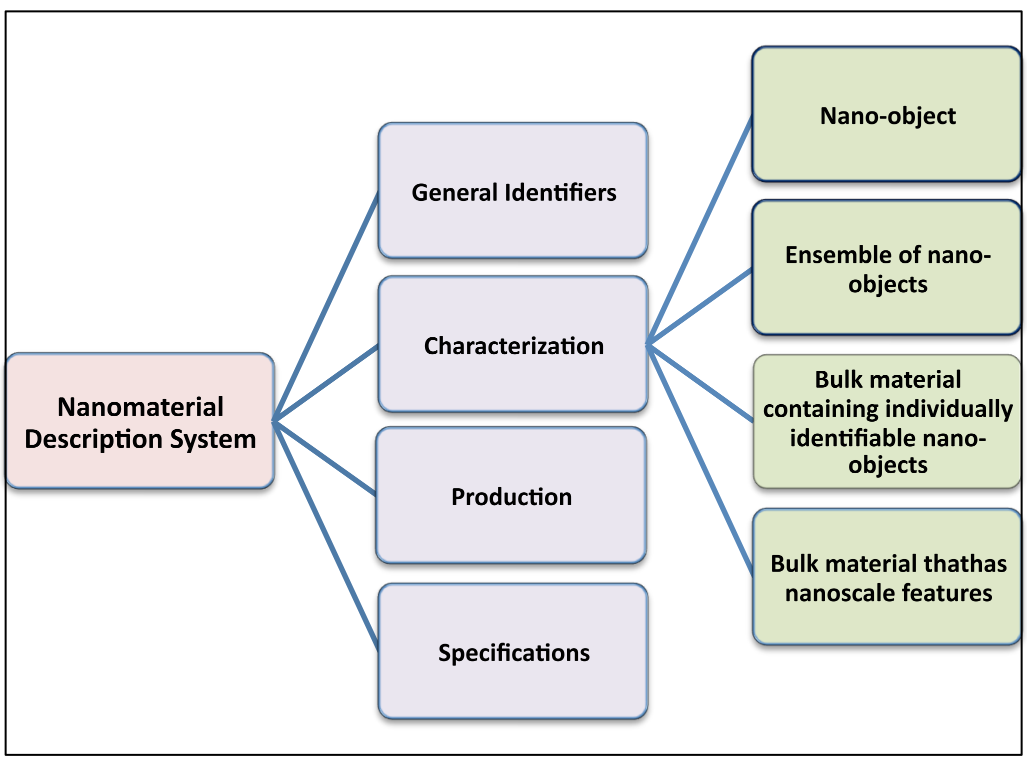
This approach was chosen so that the majority of the terms and concepts used in the description system are readily understandable to the scientists, technologists, and lay persons involved in nanotechnology. It is anticipated that the description system will be used by many different users groups, including informatics experts who design and implement data and information resources using the latest informatics tools such as information modeling, ontologies, and semantic web technology. Such efforts will likely uncover some ambiguities and redundancies, and that knowledge can be fed back into updates and evolution of this description system.

The basic premise behind the Uniform Description System is that unlike individual molecules, a nanomaterial cannot be uniquely specified by a simple, or even complex, name. Further, the description systems developed for metals, alloys, ceramics, polymers, and composites are also in an incomplete state for nanomaterials because of size, surface, shape, and other effects that significantly influence their properties. While simplistic terms such as “carbon nanotubes” or “quantum dot” convey important information, identification of a specific nanomaterial requires more. Instead, for complete specificity, all relevant information categories need to be used. Many situations require this level of specificity including the development of regulations, standards, purchasing, and testing.

One can imagine in the future a numbering system that traces back to specific values of the descriptors included in the information categories of the UDS.

# IV. Framework

The first step in the development of the UDS was a survey of a large variety of user communities as to their needs, as well as the convening of a series of interactive workshops to obtain consensus on the approach. There were also interactions with standards committees such as ISO Technical Committee 229 Nanotechnologies [2] and ASTM Committee E56 on Nanotechnology [3], as well as groups such as the OECD Working Party on Manufactured Nanomaterials [4]. Based on this preliminary work, a Framework of the information used by different disciplines in their nanomaterials work was created. The Framework integrated existing approaches that have focused on specific detailed aspects of nanomaterials, such as size, shape, structure, etc. The Framework is shown in Figure 1.



The final Framework, www.codata.org/nanomaterials , defined four major information categories used to describe nanomaterials as shown in Table 1.

| Table 1. Major Information Categories Used to Describe a Nanomaterial | |
|---|---|
| **Information Category** | **Description** |
| ***General Identifiers*** | The general terms used to name and classify a nanomaterial |
| ***Characterization*** | A set of measurement results that taken together uniquely describes the physical, chemical, structural and other characteristics of a nanomaterial |
| ***Production*** | A set of general and specific information that describes the production of a nanomaterial. The production of a nanomaterial is assumed to have a distinct initial phase followed by one or more post-production phases. |
| ***Specification*** | A set of detailed information about specification documentation according to which a nanomaterial has been produced or documented. |

**Table 1. Major information categories used to describe a nanomaterial**

Each of these information categories contains numerous subcategories that in turn contain the descriptors that provide the detailed information and data comprising a complete 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 UDS identifies the various types of information and data that can be used to describe a nanomaterial; it does not, however, prescribe which pieces of information and data must be reported; that will be determined by the reason for describing a nanomaterial, which in turn is determined by the community receiving the information and data. It should also be noted that additional descriptors may become necessary as our knowledge of the properties of nanomaterials increases.

## V. Types of nanomaterials

Throughout this document, the term *nanomaterials* is used to mean *materials on the nanoscale*. While a variety of definitions of nanomaterials exist, two international standard definitions have been adopted. This Framework is intended to be compatible with both definitions.

The ISO TC229 definition [5] 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 [6] 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 %.*

In establishing the UDS, the rich array of actual and potential nanomaterials requires considerable detail to be differentiated from one another. It is extremely useful, however, to divide nanomaterials and the objects that contain them into four major types:

1. An individual nano-object
2. An ensemble of nano-objects
    a. Identical nano-objects
    b. Different nano-objects
3. A bulk material containing individually identifiable nano-objects
4. A bulk material that has nano-scale features

Each type of nanomaterial requires slightly different sets of information to describe them completely.

It must be recognized that the distinction between bulk materials of types 3 and 4 may be difficult to determine and the use of information categories related to those types will depend on the application and discipline. The majority of "products" made from nanomaterials will primarily be of one of these types. At the same time, the functionality of nanomaterials may really take place as an individual nano-object or as an ensemble of a small number of nano-objects that have separated in use from the bulk material that originally contained it. This is especially true for bio-medical functionality.

It should be noted that the applicability of the UDS is not limited to engineered or manufactured nanomaterials but is also pertinent to naturally occurring nanomaterials. In the following sections these information categories are examined in much greater detail.

# VI. Use of the Uniform Description System

The purpose of the Uniform Description System is to allow users, regardless of discipline, type of nanomaterial, or application, to use a common method for accurately describing a nanomaterial. Possible uses include the following.

**Nanoinformatics:** As researchers improve the quality and reproducibility of property measurements on nanomaterials, many groups will build data collections or measurement results. Users in turn will want to use multiple data resources to gain access to comprehensive information. The UDS provides a backbone for building the database schemas and ontologies that are at the core of a nanoinformatics resource so that information from different resources can be compared and contrasted correctly.

**Regulatory actions:** The UDS provides a methodology that allows regulators to define more accurately the specific nanomaterial(s) being regulated. Ambiguous and ill-defined terms such as carbon nanotubes are not adequate for regulations. For example, certain forms of titanium oxide have toxic effects; other forms do not. Simply declaring titanium oxide as a species to be regulated without additional specificity of its form would be incorrect.

**Standards developers:** The UDS provides standards developers with a structure to help identify critical areas for standardization and the research needed to intelligently address those areas. For example, the description of the surface of a nano-object and the topology of an ensemble of nano-objects are areas in which no consensus approach exists to describe the complexity of nanomaterials in those areas.

**Correlation of properties with nanomaterial features:** The descriptors in the UDS can be considered as independent variables that affect in some way the properties of a nanomaterial. To be able to predict properties, one must identify and understand all the major variables that affect that property. The UDS provides a rigorous framework for systematically identifying and reporting the relationship between a feature and a property, which is of particular importance to health, safety, and environmental issues.

**Researchers:** As new nanomaterials are discovered and formed, an accurate description is necessary so future researchers are able to perform future studies on the same nanomaterial. Already the scientific literature is being written with ambiguities present. One that commonly occurs is the use of the @ symbol to indicate both when a molecule or nano-object is inside or attached to a second molecule or nano-object. The UDS provides guidance to journals to avoid such ambiguities in the literature.

**Purchase of nanomaterials:** The complexity of nanomaterials precludes their specification by a simple name or formula. Purchasers of nanomaterials want to know exactly what they are getting, and providers of nanomaterials want to be able to clearly state what they are providing. The UDS provides a system to meet both needs.

**Prediction of properties and evaluation of materials for use:** The adoption of nanomaterials for use in products and other applications depends on the availability of reliable data about their performance under specified conditions. The UDS provides a mechanism for consistent reporting of data as well as the use of data from multiple sources in design and performance prediction software.

# VII. General identifiers

As with all scientific fields, the practitioners create formal and informal terminology to refer to aspects of the objects that are of interest, especially to be able to aggregate items of interest into classes. Such identifiers include

- Common or informal names and identifiers
- Formal names and identifiers, as determined by rules or as assigned by an authority
- Informal classifications based on one or more features
- Formal classifications as determined by rules or as assigned by an authority

## A. Common or informal names and identifiers

Most physical objects have multiple names that have evolved through needs to name something that is being discussed. Common and informal names for all types of nanomaterials are no exception, and any implementation of the UDS needs to be able to include such names. One simple example is the multiplicity of acronyms used for single walled carbon nanotubes, i.e. CNT, SWNT, and SWCNT.

## B. Formal names and identifiers, as determined by rules or as assigned by an authority

Formal chemical names can be assigned to chemical moieties through a series of rules established by authorities such as the International Union of Pure and Applied Chemistry [7] or by a commercial service such as the Chemical Abstract Services [8]. A number of similar systems are used for metals, alloys, polymers, and other engineering materials. Similar systems will be established for various nanomaterials in the future, though it is likely that there will be multiple systems.

## C. Informal classifications based on one or more features

Most physical objects are put into informal classes based on one of more features, i.e. size, shape, content, functionality, etc. For nano-objects, classes commonly used are based on form (nanotubes), size (quantum dots), content (graphene), and many more. Such classes arise informally and have no rigorous definition.

## D. Formal classifications as determined by rules or as assigned by an authority

The proliferation of nanomaterials has led to the more formal assignment of classes by authorities such as ISO and other standard development organizations, commercial groups, regulators, and other organizations. These classes are based on form, size, content, and other aspects, with clearly (hopefully) definition for inclusion or exclusion. Table 2 includes some classes as defined and approved by ISO TC 229 on Nanotechnology. Of particular interest is the first entry *Nano-tree* that presents a broad classification scheme for nanomaterials.

**Table 2. Examples of Formal Classes Approved by ISO TC 229**

| Classification Term | Definition (without notes) | ISO Document |
|---|---|---|
| Nano-tree | Differentiates nanomaterials in terms of their internal/external structures, chemical nature, and physical, mechanical, biological, and other properties. | ISO/TR 11360:2010(en) |
| Nanoparticle | Nano-object with all three external dimensions in the nanoscale | ISO/TS 27687:2008(en), 4.1 |
| Nanoplate | Nano-object with one external dimension in the nanoscale and the two other external dimensions significantly larger | ISO/TS 27687:2008(en), 4.2 |
| Nanofibre | Nano-object with two similar external dimensions in the nanoscale and the third dimension significantly larger | ISO/TS 27687:2008(en), 4.3 |
| Nanotube | Hollow nanofibre | ISO/TS 80004-3:2011(en), 2.6 |
| Nanorod | Solid nanofibre | ISO/TS 80004-3:2011(en), 2.7 |
| Nanowire | Electrically conducting or semi-conducting nanofibre | ISO/TS 27687:2008(en), 4.6 |
| quantum dot | Crystalline nanoparticle that exhibits size-dependent properties due to quantum confinement effects on the electronic states | ISO/TS 27687:2008(en), 4.7 |

| | | |
|---|---|---|
| nanostructured materials | One of five types: nanostructured powder; nanocomposite; solid nanofoam; nanoporous material; fluid nanodispersion. | ISO/TS 80004-4:2011(en) |
| nano-onion | spherical nanoparticle with concentric multiple shell structure | ISO/TS 80004-3:2010(en), 2.8 |
| MNO | nano-object intentionally produced for commercial purposes to have specific properties or composition | ISO/TS 13830:2013(en), 3.4 |
| stealth nano-object | nano-object specifically designed to avoid detection or rejection by the body's defence system | ISO/TS 80004-7:2011(en), 4.1 |
| manufactured nan o-object | nano-object intentionally produced for commercial purposes to have specific properties or composition | ISO/TS 12805:2011(en), 3.3 |
| PCMNO | products in which manufactured nano-objects are intentionally added, attached or embedded | ISO/TS 13830:2013(en), 3.9 |
| engineered nanoparticle | nanoparticle intentionally engineered and produced with specific properties | ISO/TR 27628:2007(en), 2.8 |
| nanoaerosol | aerosol comprised of, or consisting of, nanoparticles and nanostructured particles | ISO/TR 27628:2007(en), 2.11 |
| nanostructured particle | particle with structural features smaller than 100 nm, which may influence its physical, chemical and/or biological properties | ISO/TR 27628:2007(en), 2.13 |

**Table 2. Examples of Formal Classes Approved by ISO TC 229**

### E. Summary of General Identifiers

The general identification of objects such as nanomaterials plays an important role in any description system. These identifiers provide a convenient and efficient way to convey a set of information that is implied in a name or class name. Whether the identifiers arise from informal usage or are established for more formal reasons, implementations of the UDS must be able to include these data.

Information systems containing property data or literature references about nanomaterials will usually use these identifiers as major access points to their content. It is important to recognize the difference between formal and informal names and formal and informal classes in creating and using these information resources. In practice, the use of informal names and classes often is more common than their formal counterparts, sometimes leading to ambiguous, confusing, or even inaccurate designations that in turn hinder the location and retrieval of desired and pertinent data and information. Users and system designers need to recognize the potential problems.

## VIII. The characterization of an individual nano-object

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 12805:2011, 3.1 as "*a material with one, two or three external dimensions in the nanoscale*."

The following eight subcategories, as shown in Figure 2, comprise the characteristics of an individual nano-object are relevant for its description. In the discussion that follows, the term "nano-object" refers to an individual nano-object.

A. Shape
B. Size
C. Chemical composition
D. Physical structure
E. Crystallographic structure
F. Surface description
G. Intensive properties
H. Interactions

Some of these subcategories have well defined methods for quantifying information about their details whereas other subcategories do not, a situation that will change as new methods for characterizing aspects of nanomaterials evolves.

### A. Shape

The characterization of the geometrical 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 shapes are discovered, additional definitions are developed. The most common criterion for defining the shape of a nano-object is its general three-dimensional geometry.

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

To describe quantitatively the shape of a nano-object, several different descriptors are required as shown in Table 3.

**Table 3. Descriptors Used to Describe the Shape of a Nano-Object**

| Descriptor | Definition |
|---|---|
| **Subcategory: Shape type** | |
| Number of dimensions on nanoscale | The number of dimensions of the nano-object on the nanoscale (1 to 100 nm) |
| General shape | Common name of shape |
| ISO 229 shape name | Shape name as defined by ISO TC 229 |
| Specific shape | Shape name with qualifiers |
| Type of thickness of a nano-object with one dimension at the nanoscale | The geometrical name of the shape taken perpendicular to the thickness |
| Cross-sectional view for nano-object with two dimensions at the nanoscale | For nano-object with two dimensions at the nanoscale, the geometrical name of the cross-section taken perpendicular to the non-nanoscale dimension; Measured value |
| Number of layers (for nano-object with two or three dimensions at the nanoscale) | When relevant, the number of layers in the shape |
| Geometric regularity | Description of the geometrical regularity of the shape |

| | |
|---|---|
| **Subcategory: Shape features** | |
| Type of feature | Features that define the shape |
| Regularity of features | The regularity of those features |
| Number of features | The number of features |
| Shape symmetry | Symmetry components of the shape |

**Table 3. Descriptors Used to Describe the Shape of a Nano-Object**

### B. Size

The dimensions needed to specify the size (internal and external dimensions) of different nano-objects vary according to the shape. In addition, some shapes 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 shape would have a well-defined set of size measurements to be reported so that property-size correlations could be made.

To describe the size of a nano-object, several descriptors are required, as defined in Table 4.

| **Table 4. Descriptors Used to Describe the Size of a Nano-Object** | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Applicable dimensions** | |
| Names of dimensions | Names of appropriate dimensions for a specific shape |
| Dimensions | Measured value for each dimension |
| Type of dimension | What dimension represents: Individual measurement, calculated, average, etc. |
| How measured | Measurement method |
| | |
| **Subcategory: Derived dimensions** | |
| Aspect ratio (when applicable) | Ratio of the greatest to the least dimension; Measured value |
| Maximum virtual diameter | Measured value |
| | |
| **Subcategory: Internal dimensions** | |
| Feature name | |
| Applicable dimension | Measured value |
| Type of dimension | |
| How measured | |

**Table 4. Descriptors Used to Describe the Size of a Nano-Object**

### C. 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 chemical moieties (functional parts of a molecule). When a nano-object has multiple internal structures, such as a core, shell, surface, or covering, the chemical composition for each structure should 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) [7] is the major international authority for chemical nomenclature and is the appropriate body to try to extend current chemical nomenclature and bonding terminology 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 also 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.

The chemical composition of a nano-object uses a number of descriptors as shown in Table 5.

**Table 5. Descriptors Used to Specify the Chemical Composition of a Nano-Object**

| Descriptor | Definition |
|---|---|
| **Subcategory: Atomic Composition** | |
| Atoms present | |
| Percentage type | Basis of the percentage: atomic; mass |
| Percentage | Measured value |
| Type of composition | What atomic composition represents: Individual measurement, calculated, average, etc. |
| How measured | Measurement method |
| | |
| **Subcategory: Molecular Composition** | |
| Molecules present | |
| Molecular formula | |
| Molecular name | |
| Structural formula | |
| CAS Registry Number | |
| IUPAC InChI | |
| Percentage type | Basis of the percentage: atomic; mass |
| Percentage | Measured value |
| Type of percentage | What the percentage represents: Individual measurement, calculated, average, etc. |
| How measured | |
| | |
| **Subcategory: Chemical Moieties** | |
| Moieties present | |
| Moiety molecular formula | |
| Moiety molecular name | |
| Moiety structural formula | |
| CAS Registry Number | |
| IUPAC InChI | |
| Percentage type | Basis of the percentage: atomic; mass |

| | |
|---|---|
| Percentage | Measured value |
| Type of percentage | What the percentage represents: Individual measurement, calculated, average, etc. |
| How measured | |

**Table 5. Descriptors Used to Specify the Chemical Composition of a Nano-Object**

## D. Physical Structure

Nano-objects can have internal structures depending on their complexity. Because nano-objects take so many different shapes, and sizes, many different physical structure models are possible. Many nano-objects are layered, contain inhomogeneities, and features such a holes, protuberances, and appendages. 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. Some nano-objects are synthesized to have specific pore sizes, e.g., for catalytic purposes. The description of structural defects and impurities, whether intentional or unintentional, should include details of the amount, identity, and location of each defect or impurity.

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

The physical structure of a nano-object uses a number of descriptors as shown in Table 6.

**Table 6. Descriptors Used to Specify the Physical Structure of a Nano-Object**

| Descriptor | Definition |
|---|---|
| **Subcategory: Layers** | |
| Number of layers | |
| Order of layers | |
| Extent of layers | |
| Composition of layers | Measured value |
| Thickness of layers | Measured value |
| | |
| **Subcategory: Shell structures** | |
| Number of shells | |
| Order of shells | |
| Composition of shells | Measured value |
| Thickness of layers | Measured value |
| Uniformity of layers | Measured value |
| | |
| **Subcategory: Physical features** | |
| Types of feature | Holes, protuberances, appendages, end cap |
| Location of feature | |
| Geometry of feature | |
| Regularity of feature | |
| | |
| **Subcategory: Defects** | |
| Type of defect | |
| Geometry of defect | |

| | |
|---|---|
| Regularity of defect | |
| | |
| **Subcategory: Entrapment** | |
| Entrapped species | |
| Type of entrapment | |
| | |
| **Subcategory: Additions** | |
| Type of addition | Corona, single entity |
| Composition of addition | Measured value |
| Geometry of addition | |
| | |

**Table 6. Descriptors Used to Specify the Physical Structure of a Nano-Object**

## E. Crystallographic Structure

The crystallographic structure of nano-objects is very important. Nano-objects can have multiple physical structures within it with different crystal structures and can be amorphous, polycrystalline, or crystalline. When the physical structure of a nano-object has multiple components, layers, etc., each distinct region can have a different crystallographic structure. 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. Subcategories and descriptors for crystallographic structure of a nano-object are given in Table 7.

| **Table 7. Descriptors Used to Specify the Crystal Structure of a Nano-Object** | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Physical structure identification** | |
| Structure name | |
| Structure type | |
| Structure location | |
| | |
| **Subcategory: Unit cell information** | |
| Lattice type | |
| Brevais lattice | |
| Space group | |
| Miller indices | |
| | |
| **Subcategory: Basic unit cell parameters** | |
| Cell length a | Measured value |
| Cell length b | Measured value |
| Cell length c | Measured value |
| Cell angle alpha | Measured value |
| Cell angle beta | Measured value |
| Cell angle gamma | Measured value |
| Cell volume) | Measured value |
| Cell measurement temperature | Measured value |

**Table 7. Descriptors Used to Specify the Crystal Structure of a Nano-Object**

## F. Surface Description

Structured surfaces on the nanoscale are 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 it 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, and that description needs to include surface charge and surface attachments.

The surface description structure of a nano-object uses a number of descriptors as shown in Table 8.

| Table 8. Descriptors Used to Describe the Surface of a Nano-Object | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: General surface description** | |
| Regularity of the surface | |
| Cleanliness of surface | |
| | |
| **Subcategory: Surface geometry** | |
| Topological variations | Nano-scale topographic variations along one dimension or two dimensions in the plane of a nanoplate, along the axis of a nanorod, around the periphery of a nanorod, or on the surface of a nanoparticle. |
| Periodicity of variations | Periodic or random along either one or two dimensions of the nanoplate's plane or in the dimensions mentioned for a nanorod or a nanoparticle; more generally the variations may be random with some specified correlation length. |
| Specific surface area | Measured value |
| How measured | |
| Surface steps | |
| | |
| **Subcategory: Surface Electronic properties** | |
| Surface charge | |
| Charge distribution | Measured value |
| How measured | |
| | |
| **Subcategory: Other surface properties** | |
| Property name | Wettability; phononic; optical; color; other |
| Property value | Measured value |
| How measured | |

**Table 8. Descriptors Used to Describe the Surface of a Nano-Object**

## G. Intensive Properties

Intensive properties for macro-materials are those properties that are normally independent of the amount (mass) and shape of the material, e.g. melting point, thermal expansion coefficient, thermal conductivity, electrical conductivity. When any of the dimensions of a material, however, are on the nanoscale, many of the properties that are intensive on the micro and macro scale are highly dependent on the dimensions of the material. All the electronic, photonic, plasmonic, phononic, and similar properties of a nanomaterial are affected by its quantum states, thereby affecting and changing all its intrinsic properties whether the nanomaterial ha one, two, or three dimensions.

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

The reporting of intensive properties of a nano-object uses a number of descriptors as shown in Table 9.

| **Table 9. Descriptors Used for the Intensive Properties of a Nano-Object** | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Intensive Property** | |
| Property type | Elastic, electrical, optical, other |
| Property name | |
| Property value | Measured value |
| Measurement or calculational method | |
| Measurement details | |
| Calculational details | |

**Table 9. Descriptors Used for the Intensive Properties of a Nano-Object**

## H. Interactions

The interactions of a nano-object are important characteristics and as nanomaterials in general are quite reactive. Interactions can be classified in a number of different ways depending on whether the interactions are purely chemical, physical, or biological in nature, or a combination thereof.

The reporting of the interactions of a nano-object uses a number of descriptors as shown in Table 10.

| **Table 10. Descriptors Used for the Interactions of a Nano-Object** | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Interactions** | |
| Interaction type | Physical, chemical, biological |
| Interaction description | |
| Interaction conditions | |
| Interaction media | |
| Interaction result | Measured value |
| Interacting species | |
| Species concentration | Measured value |
| Interaction rate(s) | Measured value |
| Measurement method | |
| Measurement details | |

**Table 10. Descriptors Used for the Interactions of a Nano-Object**

# IX. The Characterization of an Ensemble of Nano-objects

Perhaps the most important type of nanomaterials from the point of actual applications is an ensemble of nano-objects, created either deliberately or through chance interactions. In most cases, the reactivity of individual nano-objects means that on a practical scale, it is difficult to produce, manipulate, and use an individual nano-object in isolation of all other nano-objects. Clearly there are exceptions when one considers applications such as are being explored in the manipulation of quantum dots for creating qubits for quantum computing applications.

An ensemble of nano-objects may be homogeneous, composed of one type of nano-object or heterogeneous, composed on two or more different types of nano-objects. Both ensemble types are characterized in the same manner, using the eight categories of information listed below.

A. Composition
B. Physical Structure
C. Interfaces
D. Surface
E. Size Distribution
F. Interactions
G. Defining Properties
H. Stability
I. Topology

An ensemble is differentiated from the third and fourth types of nanomaterial in that it contains only nano-objects, whereas the other types of nanomaterials are bulk materials containing nanomaterials or bulk materials with features on the nanoscale. Because of the wide diversity of possible ensembles, considerable thought must be given to the details of accurately describing an ensemble, and in many situations, the description will be made on the basis of an *average* or *representative* ensemble rather than each individual ensemble. The implications of this approach are significant. The correlation of properties with ensemble features may be difficult. In a distribution of ensembles, individual ensembles away from the *average* might exhibit different levels of reactivity and properties, than those that are *average*. Indeed over time, the description of a distribution of ensembles might be a new level of description for the UDS. For the present, we assume that the UDS is being used to describe one specific ensemble.

Further, there remains the ambiguity of an individual nano-object that has acquired adherents, either as a full corona or partial coverage. In these cases, using the information categories for an individual nano-object is preferred.

## A. Composition

The composition of an ensemble of nano-objects is established by specifying the nature of each type of nano-object present and the amount thereof. The homogeneity of an ensemble can range from completely homogenous, that is, comprising of identical nano-object of the same shape, size, and composition to completely inhomogeneous, that is, a random mixtures of different nano-objects that vary in terms of composition, shape, size, and other characteristics. The descriptors used for composition are given in Table 11.

| Table 11. Descriptors Used to Specify the Composition of an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Composition overview** | |
| Number of different nano-objects present | The number of different nano-objects present in the ensemble |
| List of nano-objects present | A list of nano-object present; some may be designated as primary or trace constituents |
| Homogeneity | Description of the uniformity of the constituent nano-objects in an ensemble |
| Degree of inhomogeneity | A measure of the lack of uniformity of the constituent nano-objects in an ensemble |
| **Subcategory: Nano-object description** | |
| Name | |
| Chemical formula (if applicable) | |
| Structural formula | |
| CAS Registry Number | |
| IUPAC InChI | |
| Percentage type | |
| Percentage | Measured value |
| Type | |
| How measured | |
| Other details from the UDS | |

**Table 11. Descriptors Used to Specify the Composition of an Ensemble of Nano-Objects**

## B. Physical Structure

The physical structure of an ensemble is characterized by the arrangement of the individual nano-objects within that ensemble. The structure may be totally regular, partially regular, or random, with each situation requiring different types of information. It is assumed that some of the dimensions of the ensemble could be on the micrometer ($10^{-6}$ m) scale. Because the number of nano-objects on the micro-scale could number in the millions, the structure on those dimensions is likely to be characterized qualitatively.

The concept of an ensemble of nano-objects implies that the ensemble itself has distinct boundaries that are both well-defined and detectable.

When describing a collection of objects, one needs to specify the following information:

- What objects are present?
- Where are they located in absolute geometric space?
- Are the objects regularly arranged?
- If so, what is their shape and what are the dimensions of that shape?
- Does the regularity extend in one, two, or three dimensions?
- If less than three dimensions, is the additional regularity in the other one or two dimensions?
- How are the objects associated with each other within the shape?
- If the regularity is only partial, are the non-regular portions random or regular themselves?
- If the structure is totally random, does that randomness extend in one, two, or three dimensions?

- Do the boundaries of the ensemble have the same structure as the interior of the ensemble?

The description of the composition and structure of the surface of an ensemble of nano-objects is addressed in a separate section. The descriptors for physical shape of an ensemble are given in Table 12.

| Table 12. Descriptors Used to Specify the Physical Structure of an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Physical structure overview** | |
| General shape | |
| Degree of regularity | |
| Dimensionality of regularity | |
| Completeness of regularity | |
| | |
| **Subcategory: Structure within regular shape** | |
| Shape name | |
| Shape dimensions | Measured value |
| Association of nano-objects within shape | |
| Shape boundary structure | |
| | |
| **Subcategory: Irregular shapes** | |
| Type of irregular shape | |
| Density of irregular shape | Measured value |
| Shape boundary structure | |

**Table 12. Descriptors Used to Specify the Physical Structure of an Ensemble of Nano-Objects**

## C. Interfaces

By their very nature, ensembles have a variety of interfaces: among individual nano-objects as well as among subsets within the ensemble as a whole. Characterizing the details of these interfaces can be a difficult task as the internal physical structure, as described in the last section, is usually only partially regular and usually incompletely characterized. In addition, the regularity often is in just one or two dimensions rather than three dimensions. Consequently the description of the interfaces is often qualitative rather than quantitative.

An interface within an ensemble of nano-objects is defined as the boundary between two distinct regions of an ensemble. An interface is described by its location, the two regions on either side of the boundaries, the boundary area, and the type and strength of the interaction. Clearly as the size of the interfacing region grows, the description can become more qualitative.

Greater inhomogeneity in the ensemble means the greater the number of interfaces that must be described. In many cases, the interface description is done qualitatively as the technology to examine individual interfaces deep within an ensemble do not yet exist.

Ensembles may be prepared by treating the surface or boundary of individual nano-objects. The interface description then needs to include surface preparation as well as a description of residues, accidental or intentional. The set of descriptors for interfaces is given in Table 13.

| Table 13. Descriptors Used to Specify the Interfaces within an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Interface overview** | |
| General type of interface | |
| Degree of homogeneity | |
| Interface preparation of nano-objects | |
| Number of different types of interfaces | |
| Density of interfaces | Measured value |
| | |
| **Subcategory: Description of individual interfaces** | |
| Interface name | |
| Interface dimensions | Measured value |
| Interface boundary structure | |
| Nano-objects forming interface | |
| Residues on interface | |
| How determined | |
| Intentional or random | |
| Uniformity of interface | |
| Distribution of interface | Measured value |

**Table 13. Descriptors Used to Specify the Interfaces within an Ensemble of Nano-Objects**

## D. Size Distribution

The distribution of sizes of the nano-objects within an ensemble is a key determinant of its overall properties. It may be desirable to have a very uniform size of nano-objects within an ensemble; in other situations, a wide distribution of sizes is needed. Considerable research has gone into developing technology to determine sizes across the range of nano-scales and types of nano-objects [9]. The size distribution descriptors are given in Table 14.

| Table 14. Descriptors Used to Specify the Size Distribution of Nano-Objects within an Ensemble | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Size distribution overview** | |
| Distribution of sizes | Measured value |
| Range of sizes | Measured value |
| Average size | Measured value |
| Medium size | Measured value |
| Method of determination | |
| Media in which determined | |

**Table 14. Descriptors Used to Specify the Size Distribution of Nano-Objects within an Ensemble**

## E. Interactions

The interactions of ensembles of nano-objects are important characteristics as nanomaterials in general are quite reactive. Interactions can be classified in a number of different ways depending on whether the interaction is purely chemical, physical, or biological in nature, or a combination thereof. The reporting of interactions of an ensemble of nano-objects uses a number of descriptors as shown in Table 15.

| Table 15. Descriptors Used for the Interactions of an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Interactions** | |
| Interaction type | Physical, chemical, biological, etc. |
| Interaction description | |
| Interaction conditions | |
| Interaction media | |
| Interaction result | |
| Interacting species | |
| Species concentration | |
| Interaction rate(s) | Measured value |
| Measurement method | |
| Measurement details | |

**Table 15. Descriptors Used for the Interactions of an Ensemble of Nano-Objects**

## F. Intensive Properties

Intensive properties for macro-materials are those properties that are normally independent of the amount (mass) and shape of the material, e.g. melting point, thermal expansion coefficient, thermal conductivity, electrical conductivity. When any of the dimensions of a material, however, are on the nanoscale, many of the properties that are intensive on the micro and macro scale are highly dependent on the dimensions of the material. All the electronic, photonic, plasmonic, phononic, and similar properties of a nanomaterial are affected by its quantum states, thereby affecting and changing all its intrinsic properties whether the nanomaterial ha one, two, or three dimensions.

This framework allows specification of a list of intensive properties as desired. It is anticipated that different disciplines and user communities will have different sets of intensive properties critical for describing ensembles of nano-objects in a specific context. The reporting of intensive properties of an ensemble of nano-objects uses a number of descriptors as shown in Table 16.

| Table 16. Descriptors Used for the Intensive Properties of an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Intensive Property** | |
| Property type | |
| Property value | Measured value |
| Measurement or calculational method | |
| Measurement details | |
| Calculational details | |

**Table 16. Descriptors Used for the Intensive Properties of an Ensemble of Nano-Objects**

## G. Stability

Once an ensemble of nano-objects is created, its stability is a key factor in determining the usability of that ensemble. Instability arises primarily for one of three reasons:

- An ensemble is inherently unstable and will break apart spontaneously.
- An ensemble is subjected to unexpected conditions such as temperature changes, violent motion, etc.
- An ensemble is exposed to a reactive species

The lack of stability may be expected or unexpected and these situations require different descriptions as shown in Table 17.

| Table 17. Descriptors Used for the Stability of an Ensemble of Nano-Objects | |
|---|---|
| **Descriptor** | **Definition** |
| **Subcategory: Stability Overview** | |
| Type of instability | |
| Expected or unexpected | |
| | |
| **Subcategory: Inherent instability** | |
| Name | |
| Type of decay | |
| Half-life of decay | Measured value |
| Method of monitoring | |
| Decay products | |
| | |
| **Subcategory: Reactive Instability** | |
| Name of reaction | |
| Media required | |
| Reaction products | |
| Stabilizing agent | |
| Concentration required | |
| Reaction products | |
| | |
| **Subcategory: Instability caused by change of conditions** | |
| Name of instability | |
| Condition that causes transformation | |
| Condition parameters required | |

**Table 17. Descriptors Used for the Stability of an Ensemble of Nano-Objects**

## H. Topology

Topology is the description of the overall connectivity and continuity of an ensemble of nano-objects or its components (where each component can be one or more nano-objects), or both. This includes 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 topological shape and the properties of an ensemble of nano-objects can be ascertained.

Topology by its very nature provides qualitative descriptions on nanomaterials. There are few direct applications of topology, but as is happening with molecular biology, researchers are finding situations in which functionality can be correlated to homeomorphism, that is the ability to transform one object (surface) into another without cutting or attachment. Another example might be the application of knot theory that studies linear structures that are tied together such that the ends cannot be undone. At present there is no system under development to describe systematically the topological features of an ensemble of nano-objects.

## X. A bulk material containing individually identifiable nano-objects

The Uniform Description system as discussed above is focused on the description of individual nano-objects or ensembles thereof. In many applications, however, nano-objects and ensembles of nano-objects will be placed in bulk materials, whether homogeneously and heterogeneously. When is service or during an application, the bulk material, which has most likely obtained different properties from the nano-objects or ensembles, still functions as a bulk material.

We can differentiate between two types of bulk materials: solid phase and liquid phase. In liquid bulk materials, nano-objects and their ensembles are free to move around in the liquid, with interactions with other components of the liquid changing over time. The description of the nano-objects and their ensembles can be done by using the information categories and descriptors defined above. In solid bulk materials, the nano-objects and ensembles more or less permanently locked in place and change locations slowly with respect to molecular time scales. Again the description of the nano-objects and ensembles can use the tools from above.

The question that then arises with respect to the description of this type of nanomaterial is the following:

*Does the bulk material have nano-scale features beyond those associated with the nano-objects or ensembles contained therein?*

One can define two extreme situations. The first is where individual nano-objects or ensembles -objects separate from the bulk materials during use or other application and move around as freely, outside the confines (boundaries) of the bulk material. In this case, the UDS is fully capable of the separated nano-objects, including a description of their production (i.e. by separation from the bulk material), if necessary.

The other extreme situation is that the use or application of the bulk material does not involve any separation of the nano-objects from the bulk material. In this case, the question becomes what additional information is needed to fully characterize the bulk material as including nano-objects. Aside from issues associated with the preparation of nano-objects before inclusion in the bulk material or with the production process of the bulk material with nano-objects, current systems for describing bulk materials, such as metals, alloys, ceramics, polymers, composites, food substances and others, should suffice.

Many cases between these two extremes are possible and as nanomaterials come into commerce, enhancements of the UDS may be necessary.

# XI. A bulk material that has nano-scale features

The fourth type of nanomaterials that needs to be described is a bulk material that has nanoscale features, but does not have individual nano-objects or ensembles of nano-objects. At present the UDS does not describe these materials.

# XII. Production

The production of a nanomaterial is assumed to have a distinct initial 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.

ISO TC 229 has produced ISO 80004-8:2013 which defines terminology applicable to nanomanufacturing. In addition, much effort is being made by several engineering communities to develop process models that are applicable to a wide variety of processes. As development of the Uniform Description System for nanomaterials progresses, these models need to be reviewed and utilized to the extent possible.

An initial set of descriptors for 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 important details.

The basic model of the production is as follows: A nanomaterial is produced from a set of starting materials using a specific recipe, equipment, and production technique under a given set of conditions.

The reporting of the production of a nano-object uses a number of descriptors as shown in Table 18.

**Table 18. Descriptors Used for the Production of a Nano-Object**

| Descriptor | Definition |
|---|---|
| **Subcategory: Starting materials** | |
| Number of components | |
| Component name | |
| Component number | |
| Component formula | |
| Component amount (absolute or percentage) | |
| Component source | |
| Component purity | |
| Component physical state | |

| | |
|---|---|
| **Subcategory: Recipe** | |
| Recipe name | |
| Recipe source | |
| Recipe documentation | |
| Recipe details | |
| Changes from recipe | |
| | |
| **Subcategory: Equipment** | |
| Equipment name | |
| Equipment manufacturer | |
| Equipment role | |
| Equipment set parameters | |
| Equipment model | |
| Calibration | |
| | |
| **Subcategory: Technique** | |
| General description | |
| Documentation | |
| Source | |
| Variation(s) used | |
| | |
| | |
| **Subcategory: Conditions** | |
| Temperature | |
| Media | |
| Composition | |
| Pressure | |
| Other initial set parameters | |
| Parameters monitored through production | |
| | |
| | |
| **Subcategory: Production Result** | |
| Nanomaterial produced | |
| Purity | |
| Composition | |
| Yield | |
| Physical state | |
| Date produced | |
| Location | |
| Producing organization | |
| Batch number | |
| Production documentation | |

**Table 18. The descriptors used for the production of a nano-object**

## B. Post Production History

In this subcategory, information of how a nanomaterial was subjected to initial post-production processing, stored, and transported. 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 reporting of post-production history of a nano-object uses a number of descriptors as shown in Table 19.

**Table 19. Descriptors Used for the Post-Production History of a Nano-Object**

| Descriptor | Definition |
|---|---|
| **Subcategory: Post-Production Process** | |
| Process type | Purification, storage preparation, actual storage, transportation preparation, actual transportation |
| **Subcategory: Process Recipe** | |
| Recipe name | |
| Recipe source | |
| Recipe documentation | |
| Recipe details | |
| Changes from recipe | |
| | |
| **Subcategory: Equipment** | |
| Equipment name | |
| Equipment manufacturer | |
| Equipment role | |
| Equipment set parameters | |
| Equipment model | |
| Calibration | |
| | |
| **Subcategory: Technique** | |
| General description | |
| Documentation | |
| Source | |
| Variation(s) used | |
| | |
| | |
| **Subcategory: Conditions** | |
| Temperature | |
| Media | |
| Composition | |
| Pressure | |
| Other initial set parameters | |
| Parameters monitored through production | |
| | |

| | |
|---|---|
| **Subcategory: Process Result** | |
| Nanomaterial produced | |
| Purity | |
| Composition | |
| Yield | |
| Physical state | |
| Date produced | |
| Location | |
| Producing organization | |
| Batch number | |
| Production documentation | |

**Table 19. The descriptors used for the post-production history of a nano-object**

# XIII. Specifications

Specifications are a mechanism to define in detail how a nanomaterial is produced, purchased, or delivered. A specification is important for documenting the agreement between two or more parties as to the exact nature of the nanomaterial under consideration. Specifications can be informal or formal, and are often legally binding. Informal specifications are often used in the purchase of an object. They are developed by and agreed to by the parties involved. Formal specifications are developed by some competent organization on behalf of a cohort of interested parties so that it can be referred or used by simple reference.

Specifications 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.

ISO TC 229 has developed a standard on guidance for specifying nano-objects [10] that is:

> *"In response to the failure of specifications agreed between suppliers of manufactured nano - objects and their customers to ensure delivery of material that responds consistently to downstream processing or that is capable of generating consistent performance in the final product between batches and lots.*
>
> *"This observed inconsistent performance of batches or lots of material has led to the conclusion that the cause has to be related to one or more of the following scenarios.*
>
> *"a) The specification agreed between customer and supplier does not cover all material characteristics that have an influence on performance and/or processability, or it has been interpreted differently by the customer and supplier.*
> *b) One or more material characteristic is currently being measured by an inappropriate technique.*
> *c) One or more measurement technique is being applied in an incorrect manner."*

In the case of nanomaterials, the specification itself contains well defined information about the nanomaterial and its properties, often including detailed information about production, shipping, and storage. Descriptors used in specifications are given in Table 20.

| Table 20. Descriptors Used for a Specification | |
|---|---|
| **Item** | **Definition** |
| Specification name | the name given in the specification document |
| Specification title – | title of specification document |
| Specification authority – | authority issuing specification document |
| Date of issue – | date of issue for specification document |
| Type of specification – | type of specification document [standard specification, regulation, company specification, purchase order, material list, etc.] |
| Version of specification – | version of the specification document |
| Identification number – | when the number refers back to a document or reference source that specifies the nanomaterial |

**Table 20. Descriptors used for a specification**

## References


[1] www.codata.org/nanomaterials

[2] http://www.iso.org/iso/iso_technical_committee?commid=381983

[3] http://www.astm.org/COMMITTEE/E56.htm

[4] http://www.oecd.org/science/nanosafety/

[5] ISO/TS 800004-1:2010(E)

[6] http://ec.europa.eu/environment/chemicals/nanotech/#definition

[7] http://www.iupac.org/home/publications/e-resources/nomenclature-and-terminology.html

[8] http://www.cas.org/content/chemical-substances/faqs

[9] *Considerations on a Definition of Nanomaterial for Regulatory Purposes*, Göran Lövestam, Hubert Rauscher, Gert Roebben, Birgit Sokull Klüttgen, Neil Gibson, Jean-Philippe Putaud and Hermann Stamm, Reference Report by the Joint Research Centre of the European Commission, EUR 24403 EN (ISBN 978-92-79-16014-1)

[10] ISO/TS 12805:2011(en) Nanotechnologies — Materials specifications — Guidance on specifying nano-objects

# Appendix A: Measurement Value

## A.1 Introduction

Scientific data are the result of a measurement made on an object under circumstances that are controlled as much as possible. While a wide variety of measurements are possible, they generally may be classified as one of three types: Experimental; Observational; and Calculational.

While there are similarities in how results are reported, the three types need to be described using significantly different information to describe the detailed procedures used. A number of models of measurement value results exist, many of which are more detailed than given below. Users are encouraged to use the models that most closely meet their information needs.

In the Uniform Description System for nanomaterials, the term *measured value* is simply stated to be a measurement result regardless of type is used.

## A.2 Measured Value

Regardless of how generated, in the UDS, *measured value* explicitly includes the following additional items as listed in Table 21.
.

| Table 21. The Content of a Measured Value | |
|---|---|
| **Item** | **Definition** |
| Value | The measured result |
| Number of significant figures | Number of significant figures being reported |
| Unit | The unit of the value |
| Uncertainty | Statement of uncertainty about the value |

**Table 21.The Content of a Measured Value**