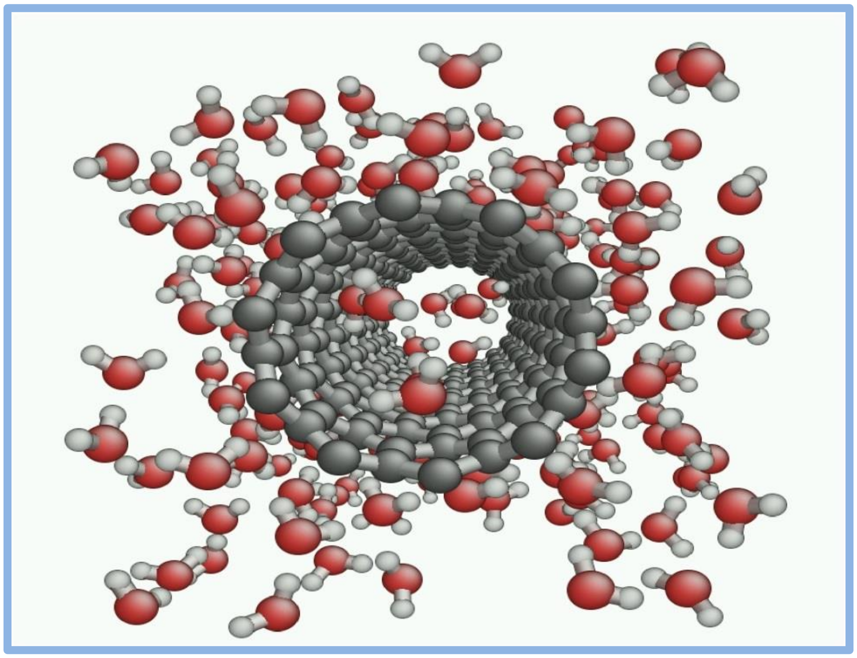
Uniform Description System for Materials on the Nanoscale



Prepared by the CODATA-VAMAS Working Group
On the Description of Nanomaterials
www.codata.org/nanomaterials

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Preface

In 2012, CODATA, the International Council for Science: Committee on Data for Science and Technology **(**www.codata.org**)**, and VAMAS, an international pre-standardization organization concerned with materials test methods **(**www.vamas.org**)**, established a joint working group to foster the development of a uniform description system for nanomaterials to address the growing diversity and complexity of nanomaterials being developed and commercialized.

The Working Group (WG) was formed following a 2012 workshop held in Paris co-sponsored by ICSU and CODATA. The international working group includes representatives from virtually every scientific and technical discipline involved in the development and use of nanomaterials, including physics, chemistry, materials science, pharmacology, toxicology, medicine, ecology, environmental science, nutrition, food science, crystallography, engineering, and more. Many international scientific unions have actively participated.

Following its work plan, the WG surveyed requirements for a description system. Over 40 responses were received that provided important insights into potential uses for a Uniform Description System for Nanomaterials (UDS). Based on the workshop and the survey, an initial draft Framework for the UDS was developed and made available for further comment and modification. That initial Framework was reviewed by the Working Group at a second workshop held in Paris in May 2013.

To continue development of the draft UDS and to obtain more complete input from all the scientific communities and variety of researchers and industries involved with nanomaterials, the CODATA-VAMAS Working Group convened a series of five international workshops:

- April 2014, North Carolina (USA)
- April 2014, Paris (France)
- September 2014, Beijing (China)
- June 2015, Rockville MD (USA)
- July 2015, Maastricht (Netherlands)

The workshops reviewed Version 1.0 in great detail from a multi-disciplinary point of view. New information categories were added and detailed subcategories and descriptors were defined. Version 2.0 is presented in the following document. The document is provided in hopes that it is directly applicable for developing data formats and ontologies, reporting research results, and other uses.

The Chairs of the WG, John Rumble, Steve Freiman, and Clayton Teague, extend our thanks to all workshop participants for their many comments, recommendations, and critiques that contributed significantly to the evolution of the UDS Framework that brought it to this latest version. Comments should be sent to nanomaterials@codata.org.

Guide to this Document

This version of the CODATA-VAMAS Uniform Description System for Materials on the Nanoscale (UDS) is divided into several parts serving different purposes and for ease of use. The following table provides a guide to the parts.

Using the UDS: Major Information Categories Used to Describe a Nanomaterial		
Title	**Part**	**Description**
Introduction, Use, Definitions, and Framework	1	Introductory material about the UDS including general definitions and the overall framework
Characterization of an individual nano-object	2	A set of measurement results that taken together uniquely characterizes the physical, chemical, structural and other characteristics of a nano-object
Characterization of a collection of nano-objects	3	A set of measurement results that taken together uniquely characterizes the physical, chemical, structural and other characteristics of a collection of nano-objects
Description of bulk materials	4	The description of the bulk materials either containing nano-objects or having features on the nanoscale
Production of nanomaterials	5	A set of general and specific data 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 of nanomaterials	6	A set of detailed information about specification documentation according to which a nanomaterial has been produced or documented
General identifiers for nanomaterials	7	The general terms used to name and classify a nanomaterial
References		
Appendix A	8	Information about the descriptors used for a measurement

Each part contains tables defining a set of descriptors with detailed definitions that can be used directly to describe individual nano-objects or collections of nano-objects. These descriptors are intended to provide guidance in describing a nanomaterial in research papers, database schemas, ontologies, regulations, modeling software, classification systems, sharing and exchanging property data.

As noted, this is Version 2.0 of the UDS. We expect that over time the UDS will be updated and expanded as users implement it in different ways. Errors, improvements, and suggestions should be sent to nanomaterials@codata.org.

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Part 1 Guide, Use, Definitions, and Framework

A. Introduction

This document is Version 2.0 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 version has been revised from Version 1.0, which in turn was based on a Framework for the UDS as previously developed by the CODATA-VAMAS WG [CODATA]. One result of this review is the division of the UDS into distinct parts as follows for clarity and ease of use.

- Part 1. Guide, use, definitions, and framework
- Part 2. Characterization of a nano-object
- Part 3. Characterization of a collection of nano-objects
- Part 4. The description of bulk materials
- Part 5. Production of nanomaterials
- Part 6. Specifications for nanomaterials
- Part 7. General identifiers for nanomaterials
- References
- Appendix A. Measurement results

One major application of the UDS is to validate database schemas, ontologies, and data deposition requirements for nanomaterial data resources. To that end, Parts 2, 3, 5, 6, and 7 should make the UDS nomenclature and structure readily accessible. The UDS has deliberately been written in the language of nanomaterials experts, with a minimum use of information and data science jargon. The scientific terminology needed to describe a nanomaterial is complex and continuing to evolve; therefore it is important that nanomaterials experts concur with this terminology.

B. Background

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 grows to describe the material accurately to the group researching it. There eventually 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 is being incorporated into products and new nanomaterials are 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 consumers 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 is under discussion 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 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 have their own terminology, yet need to communicate effectively with one another.

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

C. Definitions

Several terms are used throughout 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.*

Information category: A set or group of related descriptors that represents 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: A material with one, two, or three external dimensions in the nanoscale (as defined in ISO/TS 80004-3:2010(en), 2.2)

Collection of nano-objects: A group of two or more nano-objects

> *Note 1: A collection of nano-objects can contain identical or different nano-objects*

Note 2: The nano-objects within the collections can be associated in a variety of ways, including but not limited to direct bonding, van der Waals attraction, electrostatic interactions, or third party mediation (e.g. catalyst)

Bulk material: A solid 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 objects (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

D. Background

The approach taken herein has been to identify the broad types of information that are used throughout 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 is desired. The terms *equivalency* and *uniqueness* are described in the definitions in above.

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 are 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 inadequate 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 that in the future a numbering system will evolve that traces back to specific values of the descriptors included in the information categories of the UDS.

E. 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 are building data collections of measurement results. Users in turn want to use multiple data resources to gain access to all available information. The UDS provides a backbone for building the database schemas and ontologies that are at the core of nanoinformatics resources so that information from different resources can be compared and contrasted correctly.

In developing a data resource for nanomaterials, the required information can be divided into three major types as shown in Figure 1. A nanomaterial has a set of properties and functionalities determined under certain measurement conditions. The UDS specifies the information categories and descriptors that should be used for the description of the nanomaterials (upper left box). The UDS should be useful as data resources develop schemas and ontologies for describing a nanomaterial. The information categories and descriptors for the properties and functionalities and measurement conditions, however, are not covered by the UDS and need to be defined by other systems, schemas, or ontologies.

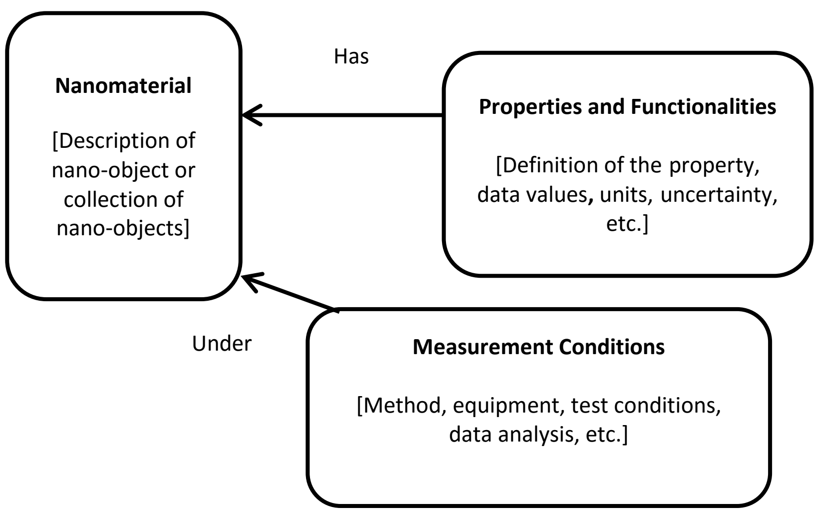

Figure 1. Types of information used to describe a nanomaterial and its properties

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

The basis for regulatory actions with respect to nanomaterials is risk assessment: Is the use of a nanomaterial in a product or food likely to cause harm to the user, the public, or the environment. These are legitimate concerns, but they need to be addressed using the best available science. Unfortunately today risk assessment is not a precise science, and assessing the real risk of nanomaterials is quite difficult. [Hunt, Krug] The testing of actual and potential nanomaterials is very challenging, first because of the large number of nanomaterials and second because small changes in a nanomaterial, such as its physical structure or surface coatings, can significantly change its interactions with biological and environmental systems, especially at the molecular and cellular level.

Consequently it is critical that in assessing risk to health and safety, i.e., unwanted and negative interactions, we are able to identify the mechanism by which these negative interactions operate. Scientifically that means understanding the factors (independent variables) about a nanomaterial that cause the negative interaction. For example, how does the chemical composition, or shape, or surface charge distribution affect the properties of a nanomaterial? Lacking detailed knowledge of cause and effect, regulators may find it convenient to issue regulations on an entire class of nanomaterials instead of a specific nanomaterial. In doing this, many nanomaterials of high value in terms of functionality or performance-enhancing capability could be unscientifically removed from commerce, a result equally undesirable as ignoring real risk.

The UDS can play an important role in facilitating scientifically sound risk assessment through its definition of the important features of a nano-object or collection of nano-objects that need to be viewed as independent variables carefully controlled during risk assessment experiments. It is critical that researchers carefully document the exact nanomaterial being tested so its behavior can be accurately correlated with specific features of the nanomaterial itself.

Indeed one of the attractions of nanomaterials is the ability to fine tune them through atomic and molecular engineering to alter their shape, size, or surfaces, which in turn alters their properties, functionalities, or reactivity. Documenting the results of that engineering accurately is one of the major goals of the UDS.

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

More importantly, as shown in Figure 2, the UDS interfaces with the test methods and protocols developed by the standards development committees. As these groups develop test methods and protocols for determining the properties and functionalities of nanomaterials, systems for describing the measurement conditions and properties must be developed to facilitate sharing of property data electronically.

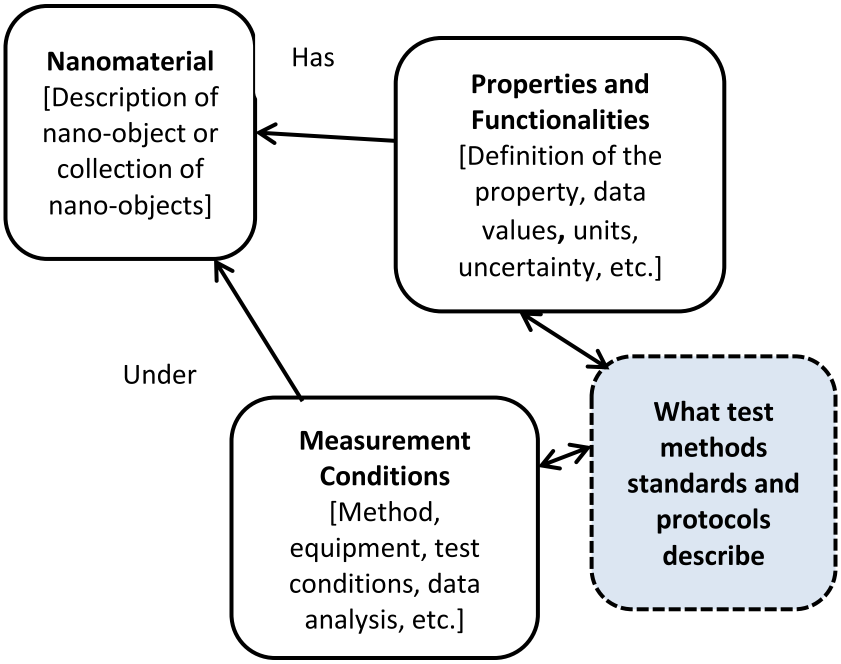

Figure 2. The relationship of test methods and protocols to the properties and functionalities of nanomaterials

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 (independent variable) and a property (dependent variable), which is of particular importance to health, safety, and environmental issues.

As discussed above under regulatory actions, the UDS has been designed to describe accurately all features of a nanomaterial so that they can be correlated with properties. This is especially true with respect to testing or research efforts that systematically vary one or more features (variables) to determine the resulting effect on a property. While this approach is important in maximizing potential positive performance (greatest strength, least reactivity, etc.), it is also critical for identifying and eliminating negative effects, such as toxicity or persistence.

Researchers: As new nanomaterials are discovered and formed, an accurate description is necessary so that future researchers are able to perform 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 should provide 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.

F. 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 major international standard definitions have been adopted. This Framework is intended to be compatible with both definitions.

The ISO TC229 definition [ISO 80004] 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 [EU Nano.] 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; each type of nanomaterial requires slightly different sets of information to describe it completely.

- An individual nano-object
- A collection of nano-objects
  - Identical nano-objects
  - Different nano-objects
- A bulk material containing individually identifiable nano-objects
- A bulk material that has nano-scale features

It must be recognized that the distinction between different types of bulk materials may be difficult to determine, and the use of information categories related to those types depend on the application and discipline. At the same time, the functionality of nanomaterials may really take place as an individual nano-object or as a collection of a small number of nano-objects that have separated in use from the bulk material that originally contained it.

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 (processed or otherwise) nanomaterials.

G. Framework

The first step in the development of the UDS was a survey of a large variety of user communities as to their need, 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 [ISO TC 229] and ASTM Committee E56 on Nanotechnology [ASTM E56] as well as groups such as the OECD Working Party on Manufactured Nanomaterials [OECD WPMN]. Based on this preliminary work, a Framework of the information used by different disciplines in their nanomaterials work was created as shown in Figure 3. The Framework integrated existing approaches that have focused on specific detailed aspects of nanomaterials, such as size, shape, structure, etc. The final Framework, which is available at 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

Major Information Categories Used to Describe a Nanomaterial	
Information Category	**Description**
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
General Identifiers	The general terms used to name and classify a nanomaterial

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

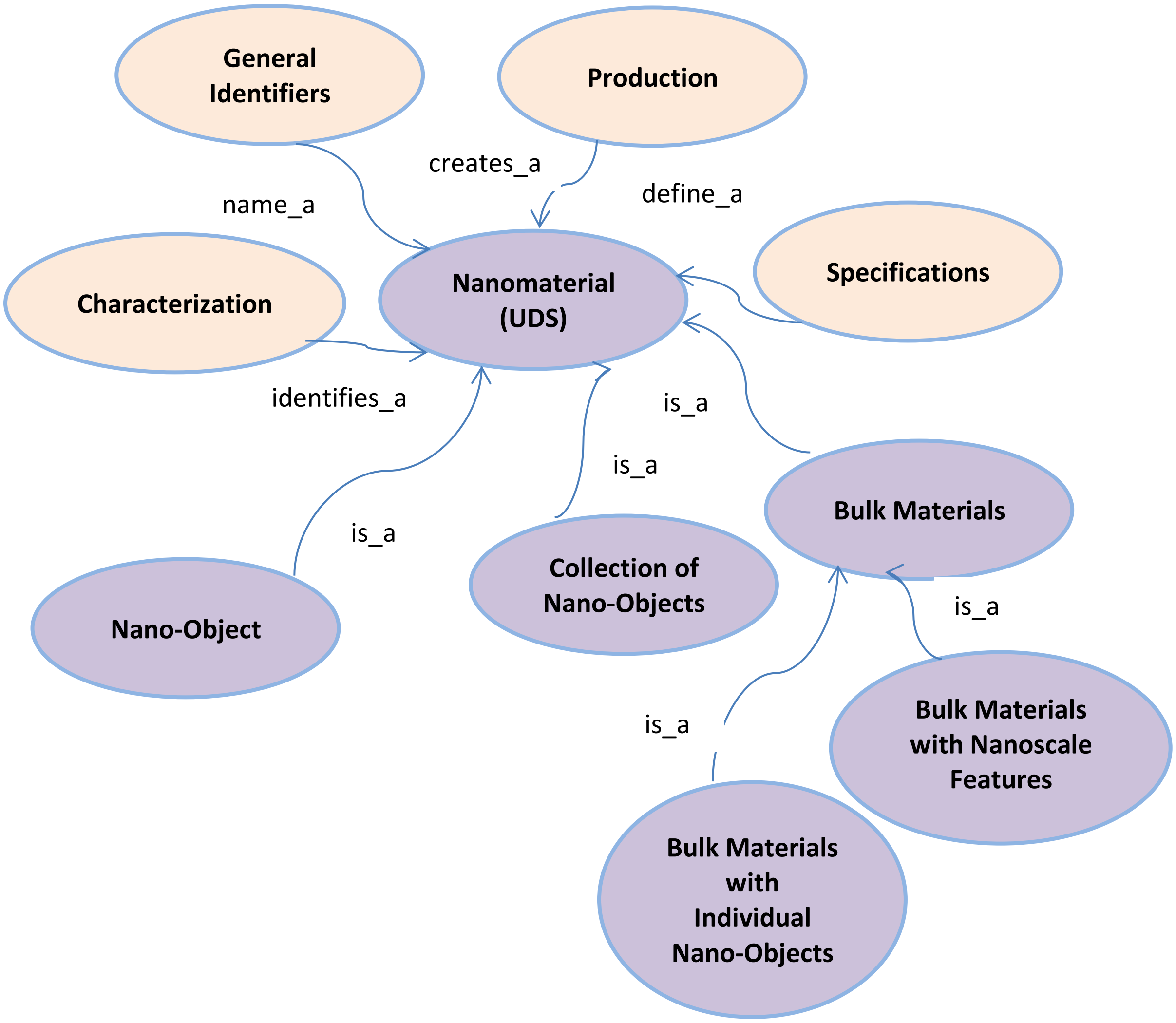

Figure 3. Framework for a uniform description system for nanomaterials

Part 2: The Description of a Nano-Object

A. 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 80004:1 as "*a material with one, two or three external dimensions in the nanoscale*."

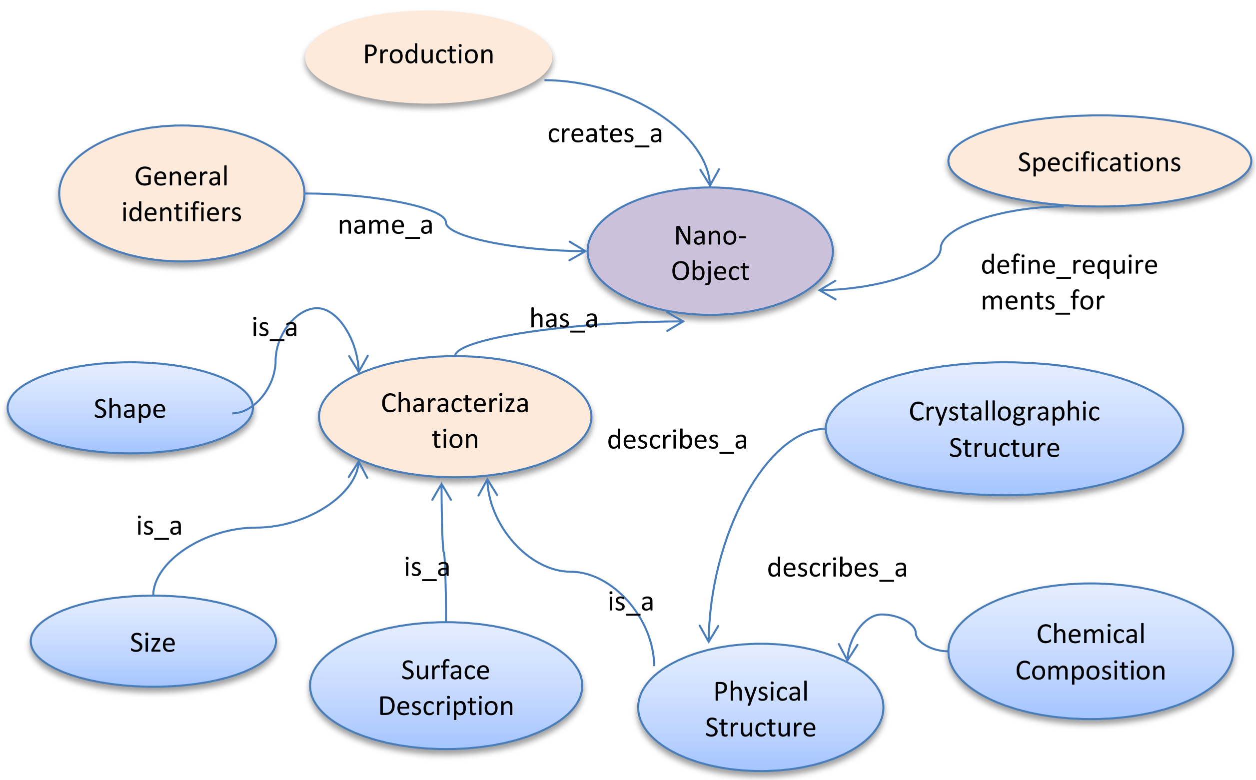

Figure 4. Information categories for describing an individual nano-object

The following six information subcategories, as shaded in Figure 4, comprise the characteristics of an individual nano-object relevant for its description. In the discussion that follows, the term "nano-object" always refers to an individual nano-object.

A. Shape
B. Size
C. Physical structure
D. Chemical composition
E. Crystallographic structure

F. Surface description

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.

B. 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, or shape type (Table 19). ISO TC 229 has defined several common shape types including: nanoparticle, nanorod, nanotube, nanoplate, and nanocone. It is anticipated that ISO TC 229 will continue to standardize the terminology associated with the shape type of newly discovered nano-objects.

For shapes with more numerous features, there is provision for enumerating and describing those features. It has been shown useful to define some quantitative measures of shape, including *aspect ratio*, or sharpness, that reflects the fiber- or rod-like nature of a nano-object, *flatness*, or the lack of unevenness of a plate-like nano-object, and sphericity that provide an indication of how spherical is a nano-object.

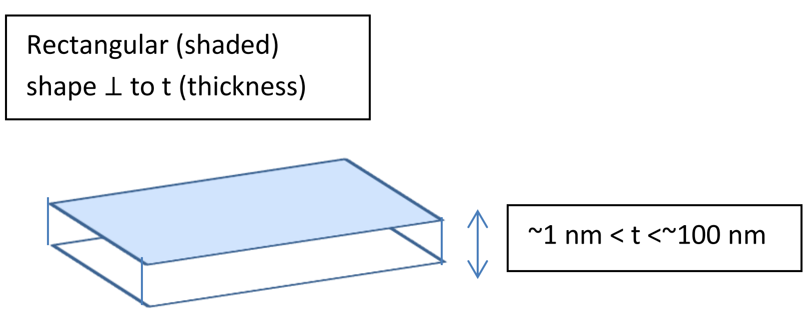

Figure 5. Geometrical shape of a nano-object with one dimension at the nanoscale

The descriptors required to describe quantitatively the shape of a nano-object are given in Table 2.

Table 2. Descriptors for the shape of a nano-object

Descriptors for the Shape of a Nano-Object		
Descriptor	**Definition**	**Notes or Examples**
Subcategory: Shape Type		
Number of dimensions on nanoscale	The number of dimensions of the nano-object on the nanoscale (about 1 to 100 nm)	1, 2, or 3 dimensions
General shape	Common name of shape	Plate; nanotube; star; etc.
Specific shape	Qualified common shape name	Multi-walled nanotube; five-pointed star; etc.
ISO 229 shape name	Shape name as defined by ISO TC 229	For example, nanoplate; nanofiber; nanotube; nanorod; nanowire; as defined in ISO/TS 27687:2008 (en) and ISO/TS 80004 -3:2011 en) see Table 19.
Geometrical shape of a nano-object with one dimension at the nanoscale	The geometrical name of the shape taken perpendicular to the nanoscale dimension (thickness)	Rectangle; circle; etc. See Figure 5.
Geometrical cross-section shape of a 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	Hexagon; circle; square; pentagon; etc. See Figure 6.
Shape symmetry	Overall symmetry of the shape	Planar; rotational; inversion; screw overall symmetry
Symmetry components	The number of and type of symmetry components	Enumerate and identify all relevant symmetry components
Subcategory: Shape Features (recurring)		
Type of feature	A feature that occurs in the shape	For example, points of a star
Regularity of feature	The regularity of that feature	e.g. Are all points, the same; if not, can they be grouped into logical categories?
Number of features	The number of occurrences of the feature	Number of instances
Symmetry of feature	The symmetry of the feature	If the features are arranged symmetrically, how?
Subcategory: Quantitative Shape		
Aspect ratio	Ratio of the greatest to the least dimension	A measure of the sharpness of a nano-object; the greater the value, the sharper the nano-object; can be used for the WHO fibre dimension determination (3:1) [WHO]

Flatness	Ratio of the largest to smallest thickness dimension for a nanoplate or similar shape	A measure of the smoothness of a nano-object; the closer to a value of 1, the flatter the surface
Sphericity	Ratio of the radii drawn from the geometric center of a nano-object to closest and furthest surface feature	A measure of how spherical a nano-object is; the closer to a value of 1, the more spherical a nano-object

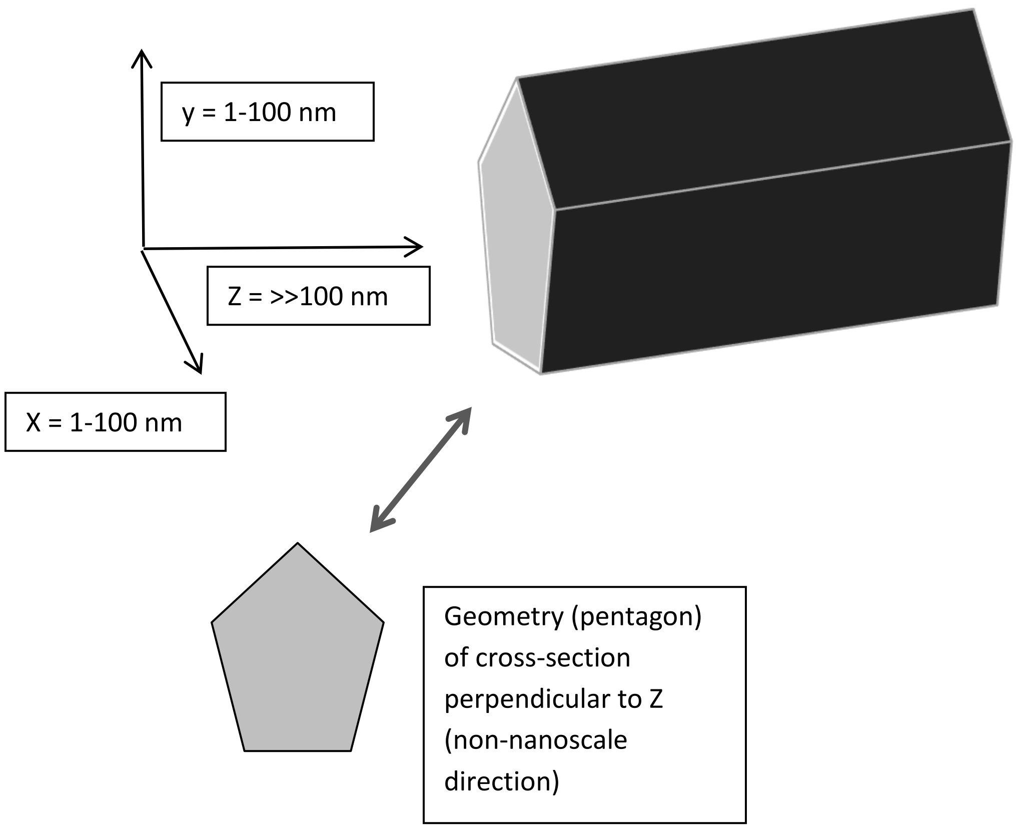

Figure 6. Geometrical cross-sectional shape of a nano-object with two dimensions at the nano-scale

C. Size

The very modifier "nano" illustrates the importance of size in describing a nano-object, yet size even on the nanoscale can vary greatly. For example, the size of a cube-shaped nano-object with all three dimensions on the nano-scale can range from 1 nm^3 to 10^6 nm^3. Similarly the surface area of a 100 nm-sided cube is 10^4 larger than a 1 nm-sided cube. As many properties of nano-objects are surface area dependent, clearly size is important. In addition to overall size and the size of internal feature, derived dimensions such as ballistic size can be reported.

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 relevant size information for a nano-object, several descriptors are required, as defined in Table 3.

Table 3. Descriptors for the size of a nano-object

Descriptors for the Size of a Nano-Object		
Descriptor	**Definition**	**Notes or Examples**
Subcategory: Applicable Dimensions		
Names of dimensions	Names of appropriate dimensions for a specific shape	Each shape has different applicable dimensions
Dimensions	Measured or computed value for each dimension	
Subcategory: Derived Dimensions		
Maximum virtual diameter	Diameter of largest sphere that can be inscribed about a nano-object while maintaining contact at two points	A measure of the "ballistic" size of a nano-object; an indication of the size of a nano-object moving in a fluid
Subcategory: Internal Dimensions		
Number of internal features	The number of internal features being reported	e.g. shape features (see Table 2) such as points of a star
Feature name	Name of each internal feature	e.g. shape features (see Table 2) such as points of a star
Names of dimensions	Names of appropriate dimensions for each individual internal feature	Each feature has different applicable dimensions
Applicable dimension	Measured or computed value for each dimension	

D. Physical Structure

Because nano-objects occur in many different shapes and sizes, a number of different physical structure models are possible; their internal structures depend on their complexity. Some nano-objects are layered or shell-like, and others contain inhomogeneities. They can have features such as holes, protuberances, and appendages. These structural components 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.

At present, no general system exists for describing the physical structure of nano-objects or of physical models that could be used as a basis for a general system. Some classes of nano-objects, such as carbon nanotubes, have had their physical structure considered in detail. For a comprehensive approach to the description of the physical structure of nanocarbon, see [Mustad]; a similar system for polymeric nano-object has been developed [Ref Tul].

All nano-objects are three-dimensional in reality, but one can effectively define a number of distinct types that have a uniform physical structure (homogeneous) and multiple physical structures (inhomogeneous), such as

- Fibrous: 1-D such as a wire or very thin rod,
- Layered: 2-D with and without homogeneity (regularity), and
- Shell-like: 3-D with and without homogeneity (regularity).

A **homogeneous** physical structure is a single phase nano-object that is uniform in any direction from the surface. [Note: the surface of a nano-object is described elsewhere in this Part.] We define **phase** as a bounded region with uniform chemical composition and crystallographic structure that can be mechanically separated from other phases. Regardless of its shape, a homogeneous nano-object has the same chemical composition and crystallographic structure throughout.

Most inhomogeneous, non-polymeric nano-objects have some regularity to their physical structures. The most common of these include layers, shells, and fibrous.

A **fibrous** nano-object can be a rod (solid) or tube (hollow) (Figure 9). A 1-D fibrous nano-object is a wire or very thin rod or tube, whose length is very much greater than its thickness and breadth. A 2-D fibrous nano-object can be solid (e.g. a short, thick nanorod) or a short single-wall nano-tube. A 3-D fibrous nano-object can be a larger solid nanorod or a multi-wall nanotube. Terms such as "sort," "long," "thin," and "thick" are difficult to define absolutely and thus are usually defined contextually.

A **layer** is defined as a two-dimensional structure with distinct edges whose third dimension is small with respect to the other two dimensions (Figure 7). A layer is either located on top of or under another layer. A layered nano-object is therefore a two-dimensional object with two or more layers, with each layer of about the same width and length, and with distinct edges.

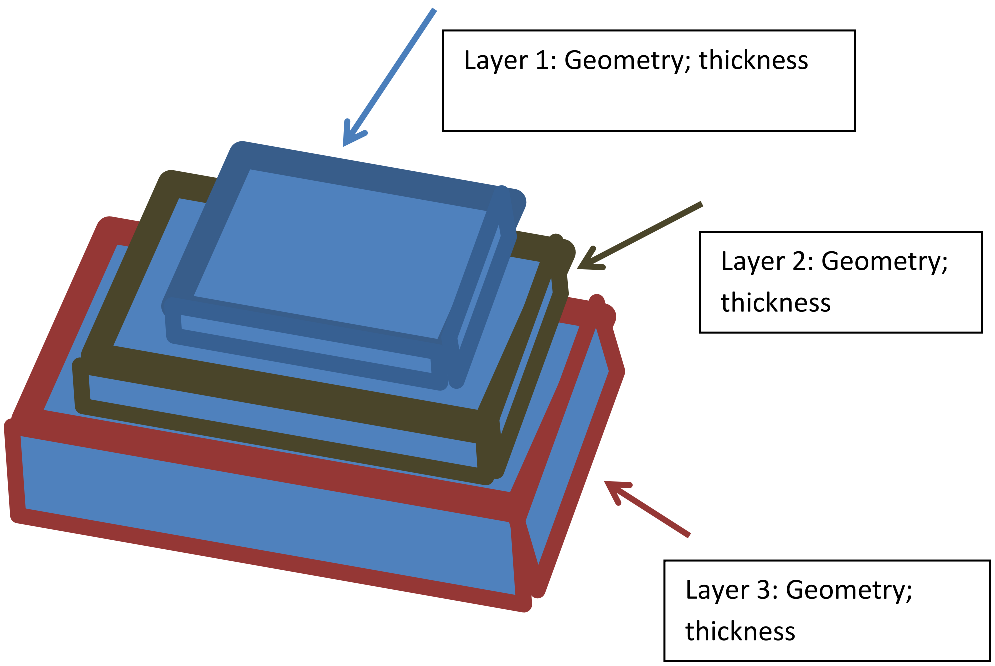

Figure 7. Schematic drawing of a layered nano-object

A **shell** is defined as a three-dimensional structure without distinct edges with one dimension (shell thickness) small with respect to the other two dimensions (Figure 8). Except for defects, a shell does not have edges. Shells may enclose or be enclosed by another shell or a solid three dimensional object, or empty space. Shells may have varying thicknesses and varying compositions. They may be static, such as the surface of a gold nanoparticle, or dynamic and transient, such as coronas found on a nano-object in biological media. The shape of a shell may or may not conform exactly to the shape of the shell or particle underneath it.

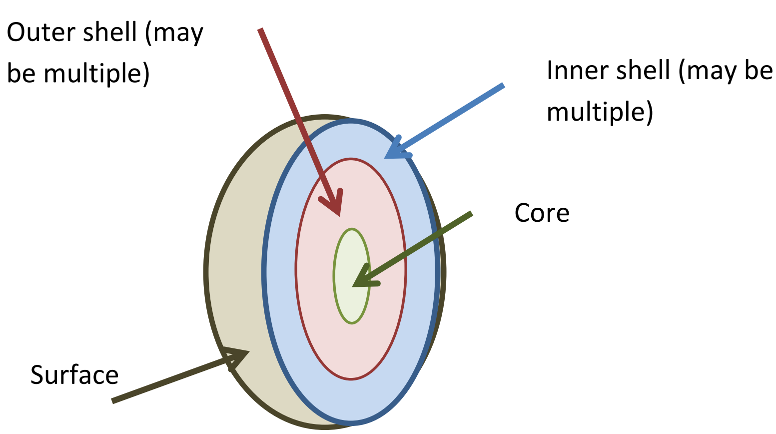

Figure 8. Schematic drawing of the cross-sectional view of a nano-object with a shell-like structure

In addition to the "regular" surfaces of its basic structure, a nano-object may have features (Figure 9), such as

- A **defect**, which is defined as a hole or other empty or missing section of the surface structure.
- An **entrapment**, which is defined as an object (atom, collections of atoms, molecules, or another nanoparticle) rigidly caught (entrapped) within a physical structure.
- An **addition**, which is defined as an object (atom, collections (layers or shells) of atoms, molecules, another nanoparticle) either tightly or loosely attached to the "regular" surface of a nano-object, but considerably smaller that the nano-objet itself.

  Note: It is subjective when to characterize an addition as only a protuberance or as something that covers an entire nano-object (layer or shell). The completeness of coverage for the addition clearly must be taken into consideration, but it is difficult to define a coverage at which an addition has become a layer or shell. Generally additions are considerably smaller than the nano-object itself.

- A **protuberance** is defined as a localized addition.

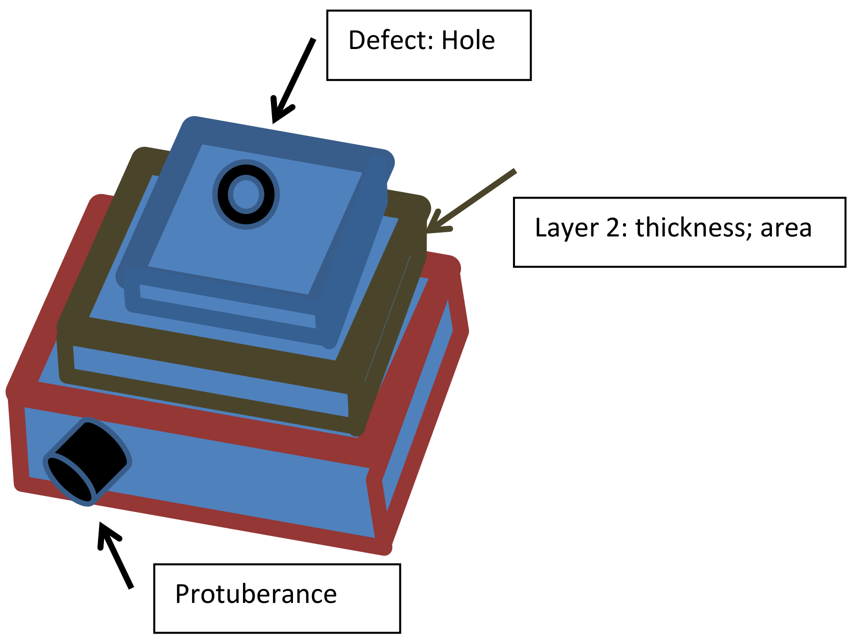

Figure 9. Schematic drawing of a defect (hole) and protuberance on a layered nano-object

The amount of detail for the physical features of a nano-object varies considerably depending on the purpose of the description, whether, for example, for research, regulation, or commercial purposes. Consequently the descriptors shown in Table 4 cover many detailed situations that may not be routinely of importance. It should be noted each component of the physical structure can have a different chemical composition and crystallographic structure (phase). Additional aspects of physical structure can be described as their importance becomes apparent.

Table 4. Descriptors for the physical structure of a nano-object

Descriptors for the Physical Structure of a Nano-Object		
Descriptor	**Definition**	**Notes and Examples**
Overall physical structure	Description of general physical structure	e.g. Homogeneous, layered, shell, other
Subcategory: Homogeneous Nano-Object		
Phase name	The phase name for homogeneous nano-object	e.g. Titanium dioxide has primary phases: rutile, anatase, and brookite
Chemical composition	The chemical composition of homogeneous nano-object	Refer to the chemical composition descriptors
Crystallographic structure	The crystallographic structure of homogeneous nano-object:	Refer to the crystallographic structure descriptors
Subcategory: Layered Nano-Object		
Number of layers	The number of layers present	May not be countable
Order of layers	The order of the layers	
Extent of layers	The physical extent of the layers	e.g. their areas or regularity
Geometry of layers	The 2-D geometrical shape of the layer	
Phase name of layers	The phase name for each layer	
Chemical composition of layers	The chemical composition of each layer	Refer to the chemical composition descriptors
Crystallographic structure of layers	The crystallographic structure of each layer	Refer to the crystallographic structure descriptors
Thickness of layers	Measured or computed value of the thickness	
Subcategory: Nano-Object with Shell Structure		
Number of shells	The number of shells present	
Order of shells	The order of the shells	
Phase name of shells	The phase name for each shell	
Chemical composition of shells	The chemical composition of each shell	Refer to the chemical composition descriptors
Crystallographic structure of shells	The crystallographic structure of each shell	Refer to the crystallographic structure descriptors
Thickness of shells	Measured or computed value of	

	the thickness value	
Uniformity of shells	Description of how uniform the shells are in terms of thickness and coverage	e.g. completeness, regularity of thickness, etc.
Subcategory: Other Physical Features		
Number of physical features	The number of physical features present	
List of physical features present	Names of the individual features	
Name of physical features	Which physical features are present	Holes, protuberances, appendages, end cap, legs, etc.
Location of each individual physical feature	Location of each individual physical feature	General or specific
Geometry of each individual physical feature	Geometrical shape of each individual physical feature	
Dimensions of each individual physical feature	Appropriate dimensions for each individual physical feature	
Regularity of the physical feature	Overall regularity of the physical features	e.g. completeness of coverage; for nano-objects with numerous other features besides layers and shells, the frequency and pattern thereof
Subcategory: Defects		
Number of defects	The number defects present	
List of defects	Names of defects present	
Location of each individual defect	Location of each individual defect	
Geometry of each individual defect	Geometrical shape of each individual defect	
Dimensions of each individual defect	Appropriate dimensions of each individual defect	
Regularity of each individual defect	Overall regularity of the location of the defects	e.g. the frequency and pattern of the defects
Subcategory: Entrapment		
Number of entrapped species	Number of species that are entrapped	
Names of entrapped species	What species is entrapped	e.g. entrapped: atoms, molecules, moieties, other nano-objects, etc.
Location of each individual entrapped species	Location of each individual entrapped species	
Chemical composition of entrapped species	The chemical composition of entrapped species	Refer to the chemical composition descriptors
Concentration of entrapped species	Amount of species entrapped	
Type of entrapment	How the species is entrapped	
Regularity of entrapment	Does entrapment repeat?	e.g. the frequency and pattern of

		the entrapped species
Subcategory: Additions		
Type of addition	Type of addition	e.g. : single molecule, other nano-object, corona, etc.
Name of addition	Name of the addition	
Species type in addition	The species comprising the addition	e.g. atoms, molecules, moieties, other nano-objects, etc.
Chemical composition of addition	The chemical composition of the addition	Refer to the chemical composition descriptors
Type of addition	How the species are added	e.g. bonding, etc.
Geometry of addition	Geometry of the addition	
Uniformity of addition	Regularity of multiple additions	e.g. completeness of coverage, uniformity of thickness, etc.

E. Chemical Composition

The chemical make-up of a nano-object is a natural way to describe that object; names such as carbon nanotubes, gold nanoparticles, and titania nanoparticles are universal terminology used by experts and the general public alike. While the chemical composition is a key descriptive category, composition subtleties are complex and important. Nano-objects are very reactive and attract many different coatings, planned and random. Many nano-objects are inhomogeneous (see the section on Physical Structure) and have non-uniform chemical composition in their different parts. Further many nano-objects are non-stoichiometric so that an accurate chemical composition is difficult to express, similar to situations found with bulk materials.

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 coating, the chemical composition for each structure must be given as appropriate. 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) [IUPAC] 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 [Bender] and paint [ASTM Paint] technology, have developed specialized terminology to describe the chemical composition of materials and need to examine if their systems for describing chemical composition need to be extended for accurate description of nanomaterials in these fields.

This information category also includes chemical structural identifiers such as the IUPAC International Chemical Identifier (InChI) [InChI], he Chemical Abstract Registry Identifier [CAS], 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 description of the chemical composition of polymers has been addressed previously [Tuominen]

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

Table 5. Descriptors for the chemical composition of a nano-object

Descriptors for the Chemical Composition of a Nano-Object		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Atomic Composition		
Number of different types of atoms present	Number of different types of atoms in the nano-object	
Atomic symbol	Symbol for each atom	
Atom name	Name of each atom	
CAS Registry Number	CAS Registry number for each atom present	
Atomic composition basis	Basis of atomic composition	e.g. percentage: number, mass
Atomic composition value	Measured or computed value of each atom	
Subcategory: Molecular Composition		
Number of different types of molecules present	Number of different types of molecules	
Molecular formula	Chemical formula for each molecule present	
Molecular name	Chemical name of each molecule present	
Structural formula	Structural formula for each molecule present	
CAS Registry Number	CAS Registry number for each molecule present	
IUPAC InChI	IUPAC InChI notation for each molecule present	
Molecular composition basis	Basis of molecular composition	e.g. percentage: number, mass
Molecular composition value	Measured or computed value of each molecule	
Subcategory: Chemical Moieties		
Number of different chemical moieties present	Number of different types of chemical moieties present	
Chemical moiety formula	Chemical formula for each chemical moiety present	
Chemical moiety name	Chemical name for each chemical moiety present	
Chemical moiety structural formula	Structural formula for each chemical moiety present	
CAS Registry Number	CAS Registry Number for each	

	chemical moiety present	
IUPAC InChI	IUPAC InChI notation for each chemical moiety present	
Moiety composition basis	Basis of moiety composition	e.g. percentage: number, mass
Moiety composition value	Measured or computed value of each moiety	

F. Crystallographic Structure

The crystallographic structure of crystalline nano-objects is very important, not only determining its phase, but also establishing some of its functionality. A nano-object can have multiple phases (physical structures) within it, each with a different crystallographic structure. The structure can be amorphous, polycrystalline, or crystalline. When the physical structure of a nano-object has multiple components, layers, etc., each phase (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 6. Additional crystallographic structure information has been defined by the International Union of Crystallography [IUCr, Bernstein].

Table 6. Descriptors for the crystal structure of a nano-object

Descriptors for the Crystal Structure of a Nano-Object		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Unit Cell Information		
Crystal system	The crystal system of the physical structure	One of seven; e.g. cubic, tetragonal, etc.
Brevais lattice	The Brevais lattice of the physical structure	One of 14; e.g. body-centered cubic, etc.
Space group	The space group	One of 230; e.g. P222 (orthorhombic)
Miller indices	The appropriate Miller indices	
Subcategory: Basic Unit Cell Parameters		
Cell length a	Cell length *a* appropriate for the crystal system value	
Cell length b	Cell length *b* appropriate for the crystal system value	
Cell length c	Cell length *c* appropriate for the crystal system value	
Cell angle alpha	Cell angle *alpha* appropriate for the crystal system value	
Cell angle beta	Cell angle *beta* appropriate for	

	the crystal system value	
Cell angle gamma	Cell angle *gamma* appropriate for the crystal system value	
Cell volume	Measured or calculated cell volume	
Cell measurement temperature	Temperature at which crystal structure data were measured	

G. Surface Description

Structured surfaces on the nanoscale are produced to have unique and useful electronic and photonic properties. Because of the reactivity of its surfaces, a nano-object has adherents on its 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 7.

Table 7. Descriptors for describing the surface of a nano-object

Descriptors for Describing the Surface of a Nano-Object		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: General Surface Description		
Overall surface structure	Description of overall surface	Regular, irregular, coated, cleaned, etc.
General reactivity of surface	Description of surface reactivity	Hydrophobic, hydrophilic, conductive
Cleanliness of surface	Description of cleanliness	Cleaned, deliberately coated, environmentally coated, etc.
Surface Treatment		
Type of surface treatment	Description of surface treatment	Oxidation, chemical, plasma assisted, etc.
Treatment process	Refer to description of post-production processing	
Resulting coating chemical composition	Use chemical composition descriptors	
Coating thickness	Measured or calculated coating thickness	
Coating completeness	Percentage coverage of the coating	
Coating uniformity	Description of uniformity or lack thereof	Gaps, thickness variability, compositional variability, geometrical variability, etc.
Subcategory: Surface Geometry		
Topological variations	Nano-scale topographic	Along one dimension or two

	variations	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 variations	Along either one or two dimensions of a nanoplate 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 or calculated specific surface area	
Surface steps	If present, description of steps and their size	Regular, irregular, dimensions, location
Subcategory: Surface Electronic Properties		
Surface charge model	Description of the model of the surface charge of a nano-object	
Type of surface charge	Sign and magnitude of surface charge	Charge sign, magnitude, full or partial
Charge distribution	Measured or calculated distribution of charge on a surface	
Subcategory: Other Surface Properties		
Color	Apparent color of the surface	
Texture	Smoothness or roughness of surface	e.g. smooth; bumpy; wavy; etc.
Reflectivity	General description of ability to reflect light	e.g. reflective; dull

Part 3. Characterization of a Collection of Nano-Objects

A. Introduction

The production and use of nanomaterials can be done on a “bottoms-up” basis resulting in a single individual nano-object, or on a “top-down” approach resulting in a number of identical, similar, or dissimilar nano-objects. These **collections of nano-objects** are the subject of this part of the UDS.

A collection of nano-objects is created either deliberately or through natural interactions and occurs during production, shipment, testing, and use. In most cases, the reactivity of individual nano-objects means that on a practical scale, it is difficult to produce, manipulate, or use an individual nano-object in isolation of all other nano-objects. 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, or the delivery of a drug via an individual nano-object.

A collection is differentiated from bulk materials with nano-objects in that a collection only contains nano-objects. There remains the ambiguity of an individual nano-object that has acquired adherents such as a full corona or partial coverage. In these cases, using the information categories for an individual nano-object is preferred. A collection of nano-objects may be homogeneous, composed of one type of nano-object, or heterogeneous, composed on two or more different types. Because of the wide diversity of possible collections, considerable thought must be given to the details of accurately describing a collection. Agglomerates and aggregates of nano-objects are considered collections.

Nano-objects rarely are produced one at a time, though “bottoms-up construction of a nano-object does happen. Consequently the initial production or manufacturing of nano-objects routinely produces collections. As nanomaterials proceed from initial manufacture to testing or use in a product, they undergo much further processing. Each step along the way is likely to produce or change the nature and characteristics of the collection.

Collections of nano-objects may vary in the number of nano-objects that are present. Examples of collections include:

- An aggregation or agglomeration of two or a small number of similar or dissimilar nano-objects
- A large number of similar or dissimilar nano-objects attached to a substrate
- A large number of (mostly) similar nano-objects produced at the same time
- A small or large number of nano-objects assembled for shipping, transport, testing, or use
- A small or large number of nano-objects assembled for inclusion in a larger amount of material

One of the major differentiators between “small” and “large” collections is whether the resulting collection can be treated as a nano-object itself. This is certainly the case when working with agglomerates and aggregates involving a very small number (2-4) of particles. We discuss these special cases at the end of this part.

Describing a collection can be done in a number of diverse ways, and different types of collections require different information for their description. In many situations, the description is made on the basis of an *average* or *representative* collection. The implications of this approach are significant. The correlation of properties with specific collection features may be difficult. In a distribution of collections, individual collections away from the *average* might exhibit significant levels of reactivity and properties different than those that are *average*. Sampling of a collection itself might change characteristics of the collection, adding to or reducing, for example, the amount of association through a change of conditions. Simple activities such as storage and transportation create dynamics that also alter the characteristics of a collection.

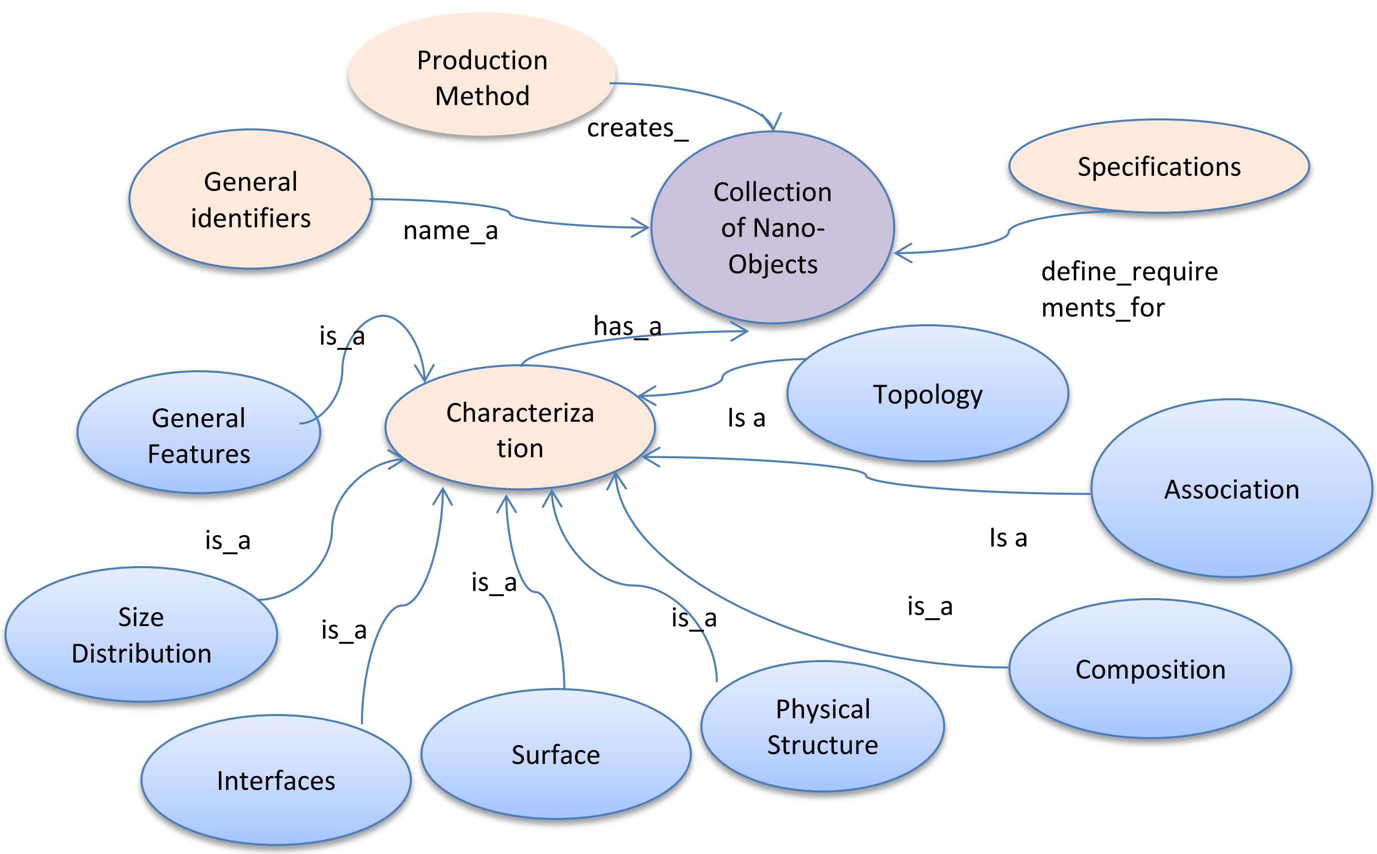

Figure 10. Schematic graphic of the information categories to describe a collection of nano-objects

Collections can be characterized using the eight categories of information listed below (Figure 10).

A. General Features
B. Composition
C. Size Distribution
D. Physical Structure
E. Association
F. Interfaces
G. Surface
H. Topology

B. General Features

In addition to specific characteristics, the description of a collection needs to include information on its general features. Descriptors used to describe the general features of a collection are given in Table 8.

Table 8. Descriptors for the general features of a collection of nano-objects

Descriptors for the General Features of a Collection of Nano-Objects		
Descriptor	**Definition**	**Examples and Notes**
Origin of collection	How was collection made?	Natural; during initial production; post-production; agglomeration; aggregation; etc.
Size of collection	General size of the collection	An individual agglomerate or aggregation; a large number of nano-objects
Homogeneity of collection	The degree of homogeneity in the collection	Number of different types of nano-objects present in the collection

C. Composition

The composition of a collection of nano-objects is established by specifying the nature of each type of nano-object present and the amount thereof. The collection can range from completely homogenous, that is, comprising identical nano-objects of the same shape, size, and composition, to completely inhomogeneous, that is, an intentional or random mixtures of different nano-objects that vary in terms of composition, shape, size, and other characteristics.

The composition of larger collections can be problematic to determine. Many production processes do not result in uniform nano-objects, especially with respect to size. The size distribution within a collection of nano-objects is the subject of the next section. For larger collections, there may be a distribution of shapes, chemical composition, physical structures (different adherents, etc.), and other features. The descriptors used for composition are given in Table 9.

Table 9. Descriptors for the composition of a collection of nano-objects

Descriptors for the Composition of a Collection of Nano-Objects		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Composition Overview		
Number of different nano-objects present	The number of different nano-objects present in the collection	Quantifies the amount of inhomogeneity
List of nano-objects present	A list of nano-objects present; they may be designated as primary or trace constituents	Identifies each type of nano-object present
Amount of each nano-object present	Concentration of the constituent nano-objects in an collection	Expressed as percent or other quantitative measure
Degree of homogeneity or inhomogeneity	A measure of the uniformity or lack thereof for the constituent nano-objects in the collection	Qualitative description of the uniformity of constituent nano-objects within the collection
Subcategory: Nano-Object Description (recurring for each constituent nano-object)		
Name	Name of constituent	From the General Identifiers as specified in that information category
Other general identifiers	Other general identifiers such as class	Multiple general identifiers descriptors as specified in that information category
Shape	Shape characteristics of constituent	Multiple shape descriptors as specified in that information category for a nano-object
Size	Size characteristics of constituent	May be described by the size distribution category in next section; if used, multiple size descriptors as specified in that information category for a nano-object
Chemical composition	Chemical composition of constituent	Multiple chemical composition descriptors as specified in that information category for a nano-object
Physical structure	Physical structure of constituent	Multiple chemical composition descriptors as specified in that information category for a nano-object
Crystallographic structure	Crystallographic structure of constituent	Multiple crystallographic structure descriptors as specified in that information category for a nano-object

Surface description	Surface description of constituent	Multiple surface description descriptors as specified in that information category for a nano-object
Production	Production method for constituent	From Production as specified in that information category
Post-production processing	Post-processing of constituent	From Post-Production Processing as specified in that information category

D. Size Distribution

The distribution of sizes of the nano-objects within a collection is an important determinant of its overall properties. It may be desirable to have a very uniform size of nano-objects within the collection; in other situations, a wide distribution of sizes is needed. Size distribution is a key element of the EU's definition of a nano-material and needs several pieces of data to report it correctly. Considerable research has gone into developing technology to determine sizes across the range of nano-scales and types of nano-objects [JRC Report]. Because different methods for determining size distribution cover different size ranges, it is important to document fully the determination method.

The size distribution descriptors are given in Table 10.

Table 10. Descriptors for the size distribution of a collection of nano-objects

Descriptors for the Size Distribution of Nano-Objects within a Collection		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Size distribution overview		
Collection sampling type	What type of sampling was done on the collection?	Individual; specific; random; average; representative, etc.
Sampling method	How was sampling done?	If average or representative collection, how was sample obtained
Distribution of sizes	The amount of each size nano-object found in the collection	List of sizes or size ranges that occur in the collection and their percentages
Range of sizes	Maximum and minimum size of constituent nano-objects	May be dependent on measurement method
Average size	Average size of nano-objects in the collection	May be dependent on measurement method
Median size	Median size of nano-objects in the collection	May be dependent on measurement method
Method of determination	Method used to determine the size distribution	Different methods lead to different results
Media in which determined	Media in which the size distribution measurement was	Measurements can be very media dependent

	made	
Other experimental variables in size distribution measurement	Equipment used and other experimental parameters, dependent on method	Dependent on measurement method

E. Physical Structure

The physical structure of a collection of nano-objects is characterized by the arrangement of the individual nano-objects within it. A collection can have no structure (totally random), for example, if simply confined in a container or in a media, or both. A collection can have a regular or partially regular structure, for instance, if the collection is attached to a substrate of some type. It is assumed that in this case, some of the dimensions of the collection could be on the micrometer (10^{-6} m) scale. Collections of nano-objects can have substructures if they are confined, such on a substrate. 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.

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

- Are the objects regularly arranged?
- If so, what is the overall 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 there partial regularity in the other one or two dimensions?
- How are the objects associated with each other within the collection?
- Are there substructures within the overall structure?
- If the regularity is only partial, are the non-regular portions randomly arranged or partially regular?
- Do the boundaries of the collection, if discernable, have the same structure as the interior of the collection?

The description of the composition and structure of the surface of a collection of nano-objects is addressed in a separate section. The descriptors for physical structure are given in Table 11. Given that many collections of nano-objects are not permanently structured, not all descriptors may be applicable.

Table 11. Descriptors for the physical structure of a collection of nano-objects

Descriptors for the Physical Structure of a Collection of Nano-Objects		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Physical Structure Overview		
Collection general shape	The overall shape of the collection, if applicable	No standard terminology has yet been developed for the shape of a collection of nano-particles; however, the terminology ISO 229 developed to describe the

		shape of an individual nano-object is useful
Collection size	The dimensions of the collection	Overall dimensions of the collection
Subcategory: Physical Structure Arrangement		
Regularity of arrangement	Arrangement of nano-objects, if regular	No standard terminology exists for regularity; may be very qualitative description
Degree of and completeness of regularity	The regularity and completeness throughout the collection	Especially relevant for collections on a substrate
Dimensionality of regularity	Number of dimensions exhibiting regularity	One-, two-, or three-dimensions
Geometrical arrangement, if any	The geometry of arrangement of the objects	If applicable
Subcategory: Structure Within Regular Shape (recurring)		
Substructure shape name	Name of a substructure shape	No standard terminology exists for describing substructures
Substructure shape dimensions	Dimensions of the substructure	For each relevant dimension
Substructure shape boundary	Description of the boundary of the substructure	

F. Association

The most important classes of association used in describing collections of nano-objects are agglomeration and aggregation. These two classes are differentiated by the strength of the bonding holding the nano-objects together. ISO TC 229 has defined for these classes as follows (underlining added).

> **Agglomerate -** Collection of weakly bound particles or aggregates or mixtures of the two where the resulting external surface area is similar to the sum of the surface areas of the individual components. The forces holding an agglomerate together are weak forces, for example van der Waals forces, or simple physical entanglement. (Source: ISO/TS 27687:2008)

> **Aggregate -** Particle comprising strongly bonded or fused particles where the resulting external surface area may be significantly smaller than the sum of calculated surface areas of the individual components. The forces holding an aggregate together are strong forces, for example covalent bonds, or those resulting from sintering or complex physical entanglement. (Source: ISO/TS 27687:2008)

It is possible to consider agglomerates and aggregates as individual nano-objects that are complex in structure and composed not of individual atoms or molecules, but of individual nano-objects. We have chosen, however, describe them as a collection, albeit one with a small number of constituents, because they have features beyond those of an individual nano-object. The descriptors for an individual nano-object can be applied to agglomerates and aggregates if useful.

Other classes of association are possible, such as attachment to a substrate and attachment to a piece of bulk material (greater than nanoscale: e.g. greater than 100 nm in all dimensions). The former class is included, but not the latter. The set of descriptors for associated nano-objects is given in Table 12.

Table 12. Descriptors for the association within a collection of nano-objects

Descriptors for Associated Nano-Objects		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Association Overview		
Nano-object association class	General type of association	Agglomeration; aggregation; attachment to substrate; other type of association
Degree of association	Complete of association	Percentage or other measure
Number of nano-objects in association	Specific number of nano-objects in the associated collection	As determined
Quality of number of nano-objects in association	Type of measurement	Measured; estimated; average; mean; etc.
Range of number of nano-objects in association	Upper and lower bounds on number of nano-objects in association	When available

G. Interfaces

An interface within a collection of nano-objects is defined as the boundary between two distinct regions. 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 becomes more qualitative. Greater inhomogeneity in a collection 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 collection does not yet exist.

Collections 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.

By their very nature, collections have a variety of interfaces among individual nano-objects as well as among subsets within the whole. Characterizing the details of these interfaces can be a difficult task as the internal physical structure, as described in the physical structure 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 dimensional. Consequently the description of the interfaces is often qualitative rather than quantitative.

The special cases of agglomeration and aggregation can also have their interfaces described using these descriptors. The set of descriptors for interfaces is given in Table 13.

Table 13. Descriptors for the interfaces within a collection of nano-objects

Descriptors for the Interfaces within a Collection of Nano-Objects		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Interface Overview		
General type of interface	Common name of type of interface	No standardized terminology available
Interface preparation of nano-objects	Method used to prepare interface for establishing the collection	If applicable
Number of different types of interfaces	Number of different types of interfaces	If applicable
Subcategory: Description of Individual Interfaces (recurring)		
Interface name	Name of specific interface	No standard names exists
Interface dimensions	Dimensions of interface	If applicable
Interface boundary structure	Structure of the interface	
Nano-objects forming interface	Name of nano-objects forming the interface	
Residues on interface	Type and amount of residue on interface	If any
Method of residue determination	Method for determining type and amount of residue	
Intentional or random	Indication of whether residue was intentionally placed or not	
Uniformity of interface	Degree of uniformity of interface	

H. Topology

Topology is the description of the overall connectivity and continuity of a collection of nano-objects or its components (where each component can be one or more nano-objects) or both, 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. The description should be done in such a way that a correlation between the topological shape and the properties of a collection 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 is 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 a collection of nano-objects.

Part 4. Bulk Materials

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 collections thereof. In many applications, however, nano-objects and collections of nano-objects are placed in bulk materials, whether homogeneously or heterogeneously. In service or during an application, the bulk material, whose properties have most likely been modified by inclusion nano-objects or collections, 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 collections are free to move around in the liquid, with interactions with other components of the liquid changing over time. In these liquid bulk materials, the description of the nano-objects and their collections can be accomplished by using the information categories and descriptors defined above. The description of the liquid bulk material thus is a sum of a description of the bulk liquid plus the description of the nano-objects and collections therein plus a description of the dynamic interactions between the bulk liquid components and the nano-objects and collections of nano-objects. As the primary components of a bulk liquid are individual molecules and molecular ions, those interactions can be quite complicated. When those molecules and molecular ions adhere to individual nano-objects, however, the UDS provides a mechanism for description.

In solid bulk materials, the nano-objects and collections are more or less permanently locked in place and change locations slowly with respect to molecular time scales. The description of the individual nano-objects and collections contained within a solid bulk material can use the UDS.

The question that then arises with respect to the description of bulk materials containing nanomaterials is the following:

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

One can define two extreme situations. The first is when individual nano-objects or collections therein separate from the bulk materials during use or other application and move around freely, outside the confines (boundaries) of the bulk material. In this situation case, the UDS can be used to describe the separated nano-objects, including a description of their production (i.e., the separation of the nano-object from the bulk material).

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 situation, the issue is what additional information is needed to fully characterize the bulk material, including contained 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 except with respect to describing how embedded nano-objects alter the behavior of the bulk material. This subject is complicated and beyond the scope of this document.

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

B. A Bulk Material Having Nano-Scale Features

There are bulk materials that have nanoscale features, but do not contain identifiable individual nano-objects or collections of nano-objects. The UDS does not describe these materials.

Part 5. Production

A. Introduction

For the purposes of the UDS, the production 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.

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. A set of descriptors for the initial production phase and a generic post-production phase are given Sections C and D below

The reactivity of individual and collections of nano-objects gives rise to questions about their **stability** under “non-reactive” conditions such as movement, temperature changes, exposure to heat, and shock (unexpected forces). These occurrences are frequent enough in the life cycle of nanomaterials as to benefit from a detail description as given in Section E.

B. Life Cycle of Nanomaterials

The reactivity of nanomaterials can caused complications for their accurate description. Specifically the reactivity of nano-objects and their collection makes it difficult to be sure of their exact composition and structure when in a medium, such as a biological or environmental fluid. Nano-objects and their collections easily are coated with bio-molecules that can dramatically alter their shape, size, and interactions. Consider the following sequence that occurs during testing as shown in Table 14.

Table 14. Sequence of steps in the testing of a nanomaterial

Test Step	Nanomaterial State	Comments
Manufactured, natural, or prepared nanomaterial	This is the substance for which users, regulators, and others want results	Almost always a collection of nano-objects
As received	In spite of precautions, changes occur during shipping and storage	Agglomeration, aggregation, reactions, degradation
As prepared for testing	Some processing takes place to restore the nanomaterial to its “original” state	Purification, reactions, etc. to reverse of shipping and storage effects
As sampled	A subset of the nanomaterial is taken for testing, hopefully fully	Standard, specified, or ad hoc procedures

	representative of the original nanomaterial	
In the test environment	Reacts with components of test media	May experience reactions, additions, alterations, including coronas, surface modification, shape and size changes, pH changes

Given this sequence of events and the substantial changes that a nano-object or collection may experience, it is unclear exactly “which” nanomaterial is being measured and how the test results are influenced by the changes at each step. Unfortunately the changes are not totally predictable. Some of the changes are caused by random events, e.g. shipping and storage events that are not predictable. Other changes results from interactions within environments that are not totally controllable, e.g. concentrations of stray bio-molecules. It should be noted that a similar sequence of events takes place for the use of a nanomaterial in an application.

In the UDS, we have taken the approach of describing the initially produced nanomaterial with post-production changes. An alternative approach, equally supported by the UDS, is to assume a nanomaterial at each step of the testing or application sequence is a separate entity and can be described using the information categories comprising the UDS. In this approach, there is no post-production processing.

C. Initial Production

The initial production information category contains the information relevant as to how a nanomaterial was first 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 the processing history information reported varies 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 more complete details.

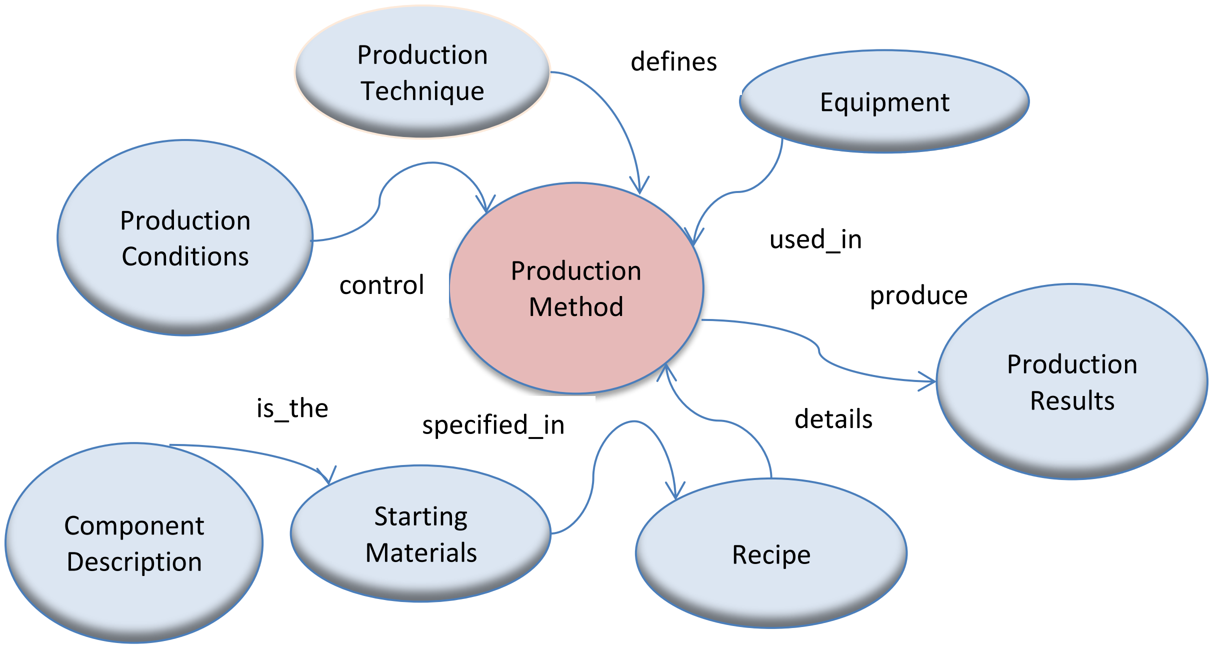

Figure 11. Schematic graphic of the production of a nanomaterial

The basic model of the production is as follows as shown in **Error! Reference source not found.**. Briefly, nanomaterial is produced from a set of starting materials using a production technique, specific recipe, and equipment under a given set of conditions. A production technique is the type of method used for producing a collection, e.g., mixing. The recipe specifies the starting materials and their actual amounts, the order of operations, and the conditions to be used. The reporting of the production of a nanomaterial uses a number of descriptors as shown in Table 15.

Table 15. Descriptors for the production of a nano-material

Descriptors for the Production of a Nano-Material		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Production Technique		
Production technique name	Name of production technique	Not standardized, but many common techniques have widely accepted names; e.g. chemical vapor deposition (CVD)
General description	Description of the production technique	Textual description
Documentation	Documentation of the production technique	When it exists; e.g. national or international standard; patent; etc.
Source	Source of the production technique	e.g. as described in the research literature
Variation(s) used	Variations from the standard production technique	Variations almost always exist

Subcategory: Equipment (recurring)		
Equipment name	Name of equipment used in production	e.g. standard or manufacturing equipment; name given by equipment manufacturer; etc.
Equipment manufacturer	Manufacturer of equipment	
Equipment model	Equipment model number	
Equipment role	Purpose of the equipment	
Equipment set parameters	Initial setting of equipment parameters	Operating parameters set and not changed during production
Calibration	Calibration details	When and how, etc.
Subcategory: Recipe		
Recipe name	Name of the recipe	Specifies starting materials, conditions, and sequence of steps
Recipe source	Source of the recipe	
Recipe documentation	Documentation of the recipe	
Recipe details	Details contained in recipe	Those not covered by starting materials or conditions
Changes from recipe	Deviations from standard recipe	
Subcategory: Starting Materials		
Number of components	The number of starting materials	
List of components used as starting materials	The names of all starting materials	Description of these uses descriptors listed below
Component Description (Recurring)		
Component name	Chemical name of the component	
Component formula	Chemical formula of component	
Structural formula	Structural formula for component	
CAS Registry Number	CAS registry number for component	
IUPAC InChI	IUPAC InChI notation for component	
Component amount (absolute or percentage)	Amount of component	Either in absolute quantity or percentage of all starting material
Component source	Source of component	Supplier, etc.
Component purity	Purity of component	Percentage basis; actual concentration; etc.
Component physical state	Physical state of component, liquid, gas, solution, etc.	
Subcategory: Conditions (not exhaustive)		
Temperature	Temperature(s) used	
Media	Media(s) used	

Media composition	Composition of media used	
Pressure	Pressure(s) used	
Other initial set parameters	Other initial conditions	
Parameters monitored through production	Parameter monitored during production	e.g., concentration, temperature, etc.
Subcategory: Production Result		
Nanomaterials produced	Nano-objects or collection of nano-objects	Use information categories for nano-objects or collection of nano-objects as appropriate
Purity	Purity of nanomaterials produced	Percentage basis; actual concentration; etc.
Composition	Amount of each nanomaterial produced	
Yield	Amount of actual production compared to theoretical amount possible	Percentage
Physical state	Physical state of nanomaterial	Gas, liquid, solid
Date produced	Date produced	
Location	Geographic or facility location of production	Details as appropriate
Producing organization	Organization that did the production	Details as appropriate
Batch number	Number of specific batch of nanomaterial	
Production documentation	Other production documentation	

D. Post Production History

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 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 nanomaterial uses a number of descriptors as shown in Table 16.

Table 16. Descriptors for the post-production history of a nanomaterial

Descriptors for the Post-Production of a Nano-Material		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Post-Production Process		
Process type	Type of post-production processing	Purification, storage preparation, actual storage, transportation

		preparation, actual transportation
Subcategory: Post-Production Technique		
Post-production technique name	Name of post-production technique	Not standardized, but many common techniques have widely accepted names; e.g. preparation for testing; for application
General description	Description of the post-production technique	Textual description
Documentation	Documentation of the post-production technique	When it exists; e.g. national or international standard; patent; etc.
Source	Source of the post-production technique	e.g. as described in the research literature
Variation(s) used	Variations from the standard post-production technique	Variations almost always exist
Subcategory: Post-Production Equipment (recurring)		
Equipment name	Name of equipment used in post-production	e.g. standard or manufacturing equipment; name given by equipment manufacturer; etc.
Equipment manufacturer	Manufacturer of equipment	
Equipment model	Equipment model number	
Equipment role	Purpose of the equipment	
Equipment set parameters	Initial setting of equipment parameters	Operating parameters set and not changed during post-production
Calibration	Calibration details	When and how, etc.
Subcategory: Post-Production Recipe		
Recipe name	Name of the recipe	Specifies starting materials, conditions, and sequence of steps
Recipe source	Source of the recipe	
Recipe documentation	Documentation of the recipe	
Recipe details	Details contained in recipe	Those not covered by starting materials or conditions
Changes from recipe	Deviations from standard recipe	
Subcategory: Post-Production Starting Materials		
Number of components	The number of post-production starting materials	
List of components used as starting materials	The names of all post-production starting materials	Description of these uses descriptors listed below
Component Description		

Component name	Chemical name of the component	
Component formula	Chemical formula of component	
Structural formula	Structural formula for component	
CAS Registry Number	CAS registry number for component	
IUPAC InChI	IUPAC InChI notation for component	
Component amount (absolute or percentage)	Amount of component	Either in absolute quantity or percentage of all starting material
Component source	Source of component	Supplier, etc.
Component purity	Purity of component	Percentage basis; actual concentration; etc.
Component physical state	Physical state of component, liquid, gas, solution, etc.	
Subcategory: Post-Production Conditions (not exhaustive)		
Temperature	Temperature(s) used	
Media	Media(s) used	
Media composition	Composition of media used	
Pressure	Pressure(s) used	
Other initial set parameters	Other initial conditions	
Parameters monitored through post-production	Parameter monitored during post-production	e.g., concentration, temperature, etc.
Subcategory: Post-production Result		
Nanomaterials produced	Nano-objects or collection of nano-objects	Use information categories for nano-objects or collection of nano-objects as appropriate
Purity	Purity of nanomaterials produced	Percentage basis; actual concentration; etc.
Composition	Amount of each nanomaterial produced	
Yield	Amount of actual post-production compared to theoretical amount possible	Percentage
Physical state	Physical state of nanomaterial	Gas, liquid, solid
Date processed	Date processed	
Location	Geographic or facility location of post-production event	Details as appropriate
Producing organization	Organization that did the post-production	Details as appropriate
Batch number	Number of specific batch of nanomaterial	
Post-production documentation	Other post-production	

	documentation	

E. Stability

One of the most important and interesting aspects of post-production processing of a collection of nano-object, or even an individual nano-object, is stability. In fact, once a collection of nano-objects is created, its stability is a key factor. Instability arises primarily for three reasons:

- The collection is inherently unstable and will break apart spontaneously,
- The collection is subjected to unexpected conditions such as temperature changes, violent motion, unanticipated reactions, etc., and
- The collection is intentionally exposed to a reactive species.

There is considerable debate about whether stability belongs in the description of a nanomaterial or as a measured property (see figure 1). It has been included in the UDS because of its importance, though it has been identified as a "special" type of post-production processing. The lack of stability may be expected or unexpected, and these situations require different descriptions as shown in Table 17.

Table 17. Descriptors for the stability of a collection of nano-objects

Descriptors for the Stability of a Collection of Nano-Objects		
Descriptor	**Definition**	**Notes and Examples**
Subcategory: Stability Overview		
Type of instability	Type of instability being described	Inherent, heat-sensitive, time-sensitive, reactive, environment sensitive, etc.
Expected or unexpected	Whether instability was expected or unexpected	
Subcategory: Inherent Instability		
Name of instability	Actual name of instability	No standard names exist
Type of decay	Mechanism of instability	No standard description of mechanisms exist
Half-life of decay	Timed half-life of instability	
Decay products	Names or types of decay products	
Subcategory: Reactive Instability		
Name of reaction	Name or type of reaction	No standard names exist
Media required	Media needed for reaction to occur	
Reaction products	Name or type of reaction products	
Stabilizing agent	Name or type of media that can be used to make collection	

	stable	
Concentration required	Amount of stabilizing agent needed	
Subcategory: Instability Caused by Change of Conditions		
Name of instability	Name or type of instability	No standard names exist
Condition that causes transformation	Cause of instability	No standard causes exist
Condition parameters required	Conditions that foster the instability	

Part 6. Specifications

A. Introduction

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 they can be referred or used by simple reference.

Specifications can also contain information about the registration of a nanomaterial in a government or, 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 and its documentation.

ISO TC 229 has developed a standard on guidance for specifying nano-objects [ISO 12805] 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 18.

Table 18. Descriptors for a specification of a nanomaterial

Descriptors for a Specification of a Nanomaterial	
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

Part 6. General Identifiers

A. Introduction

As with all scientific fields, 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 or categories. 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, and
- Formal classifications as determined by rules or as assigned by an authority.

B. Common or Informal Names and Identifiers

Most physical objects have multiple names that have evolved through the need 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.

C. 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 [IUPAC] or by a commercial service such as the Chemical Abstract Services [CAS]. A number of similar systems are used for metals, alloys, polymers, and other engineering materials. Such systems are likely to be established for various types of nanomaterials in the future though it is likely that there will be multiple systems. The timing of the establishment of a formal naming system is unclear.

D. 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 (e.g. nanotubes), size (e.g. quantum dots), content (e.g. graphene), and many more. Such classes arise informally and have no rigorous definition. The classes can be the basis for categorisation or "read-across" activities that have as a goal the correlate of properties with one or more features. When established on a sound scientific basis, such categories can be used to predict the properties of new nanomaterials, thereby reducing the amount of testing required for risk assessment or other functionality. Currently the categorisation of nanomaterials is an active field, Categories based on chemical composition, shape, size, surface properties and combinations thereof have been proposed. No categorisation scheme has yet been proven successful.

E. 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 19 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 categorisation or classification scheme for nanomaterials.

Table 19. Examples of formal classes approved by ISO TC229

Examples of Formal Classes Approved by ISO TC 229		
Classification Term	Definition (without notes)	ISO Document
Nanotree		
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-	Nano-object specifically designed to avoid	ISO/TS 80004-7:2011(en),

object	detection or rejection by the body's defence system	4.1
Manufactured nano-object	Nano-object intentionally produced for commercial purposes to have specific properties or composition	ISO/TS 12805:2011(en), 3.3
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

Classification schemes for nanomaterials are presently of great interest for regulatory purposes. These schemes can be based either on features of a nanomaterial or on a property thereof. The logic of classes based on features, such as size, chemical composition, etc., is that the feature correlates strongly with a desirable or undesirable property, especially those related to a risk, such as toxicity or environmental degradation. It should be noted that this correlation process is often referred to as "Read Across" [Ref]. Many of the proposed classification schemes are simplistic, overlooking the complexity of nanomaterials and the multi-variable dependency of a "property" such as toxicity; however, no categorisation scheme has been proven to be widely valid. Over time as the causal relationship of property to specific features is clarified, these classification schemes will become more accurate and therefore more useful.

F. 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 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.

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Appendix A: Measurement

A.1 Introduction

Scientific data are the result of measurements made on one or more objects 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 major types:

- Experimental: a situation is created in which all independent variables are controlled and measurements are made on a tangible object
- Observational: measurements are made on a situation as found in nature and few if any independent variables are controlled
- Calculational: a mathematical model is created to approximate a situation and virtual measurements are made through modeling or simulation calculations

While there are similarities in how results are reported, the three types of results need to be described using significantly different information to describe the detailed measurement procedures used.

The UDS has been designed primarily to address experimental measurements, though calculational measurements can also use the information categories and descriptors as appropriate. In the tables that contain the descriptors that comprise the UDS, many descriptors are the result of direct measurements. For example, in Table 10 on size distribution, “average size” is a descriptor. Each descriptor that contains a direct measurement can have a number of pieces of information to define the measurement result. This information includes, as shown in Figure 12.

- Measurement technique
- Equipment
- Measurement conditions
- Measurement procedures
- Analysis procedures

A number of data models and ontologies for experimental measurements have been developed and are being extended to cover more complicated measurements. [Example] It suffices here to present a general model of a measurement, to which additional detail can be added by users of the UDS.

As indicated by the text box at the bottom right of figure A.1, measurement results comprise four essential elements.

- Result (property) name
- Result (property) value
- Units
- Uncertainty

Additional information can be added, such as number of significant figures, distribution of results, averages, etc. depending on the experimental situation.

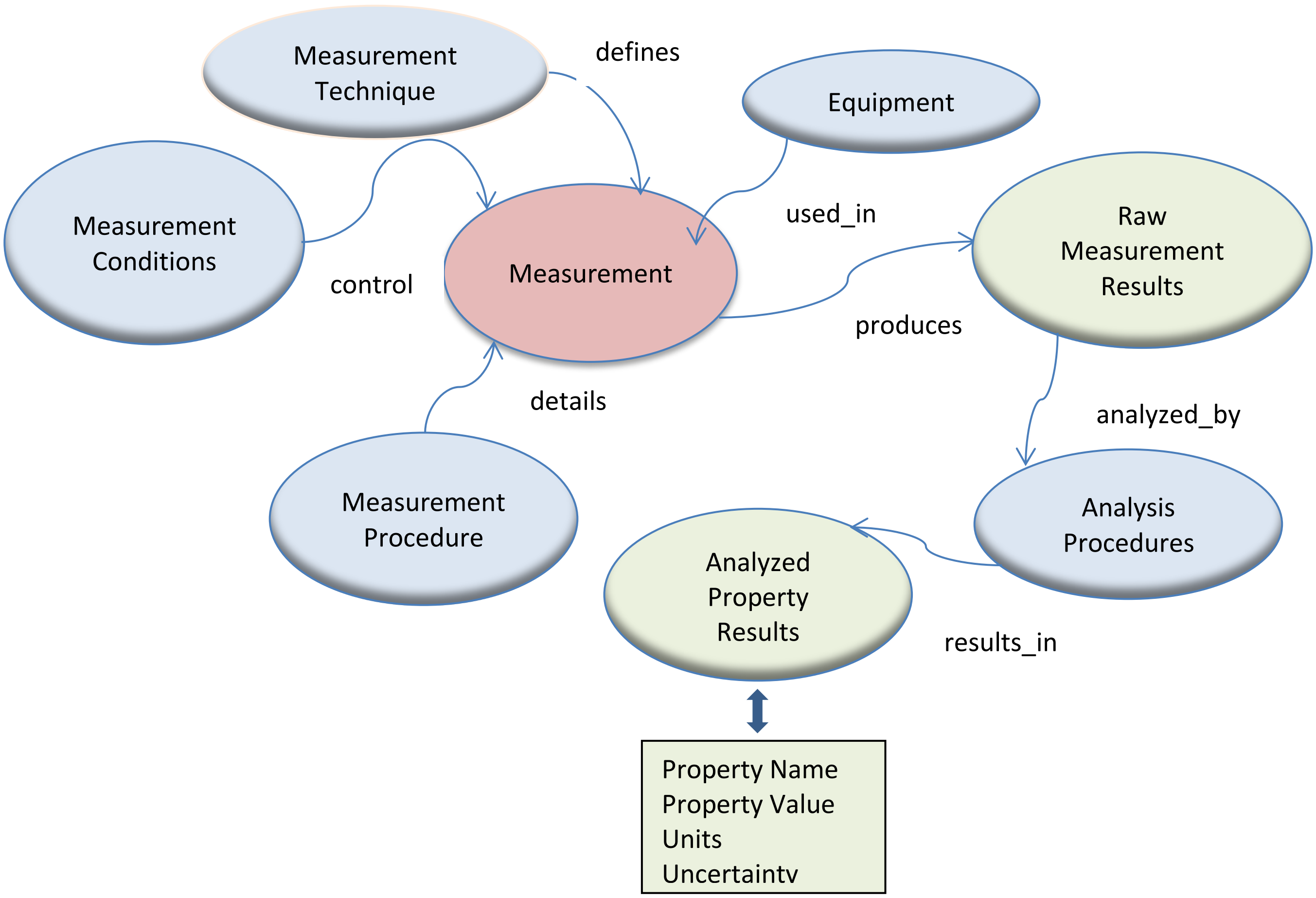

Figure 12. Schematic graphic of the information categories for a measurement