Designation: E3144 – 19

Standard Guide for Reporting the Physical and Chemical Characteristics of Nano-Objects[1]

This standard is issued under the fixed designation E3144; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This guide provides guidelines for a description system for reporting the physical and chemical characteristics of individual nano-objects. It establishes information categories and descriptors useful in describing individual nano-objects uniquely and such that the equivalency of two or more individual nano-objects can be determined according to specific criteria.

1.2 This guide is designed to be directly applicable to reporting the physical and chemical characteristics of nano-objects in every circumstance, including but not limited to reporting original research results in the archival literature, developing ontologies, database schemas, data repositories, and data reporting formats, specifying regulations, and enabling commercial activity.

1.3 This guide is applicable to naturally-occurring, engineered, and manufactured nano-objects.

1.4 One goal of the guide is to help ensure that when measurement results are reported, they are reported uniformly.

1.5 A second goal of the guide is to encourage reports on the properties and functionalities of a nano-object to include as much detail as possible about the physical and chemical characteristics of that nano-object so it is uniquely specified.

1.6 This guide does not cover the chemical reactions or reactivity of a nano-object.

1.7 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.8 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.9 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

D16 Terminology for Paint, Related Coatings, Materials, and Applications

E3172 Guide for Reporting Production Information and Data for Nano-Objects

2.2 *ISO Standards:*[3]

ISO/TS 12805:2011(en) Nanotechnologies – Materials Specifications – Guidance on Specifying Nano-Objects

ISO/TS 18158:2016(en) Workplace Air – Terminology

ISO/TS 20787:2017(en) Nanotechnologies – Aquatic Toxicity Assessment of Manufactured Nanomaterials in Saltwater Lakes using *Artemia sp. Nauplii*

ISO/TS 27687:2008(en) Nanotechnologies – Terminology and Definitions for Nano-Objects – Nanoparticle, Nanofibre and Nanoplate

ISO/TS 80004-1:2015(en) Nanotechnologies – Vocabulary – Part 1: Core Terms

ISO/TS 80004-3:2015(en) Nanotechnologies – Vocabulary – Part 3: Carbon Nano-Objects

2.3 *Other Documents:*

The Uniform Description System for Materials on the Nanoscale CODATA-VAMAS Working Group on the Description of Nanomaterials, as released on 25 May 2016[4]

[1] This guide is under the jurisdiction of ASTM Committee E56 on Nanotechnology and is the direct responsibility of Subcommittee E56.01 on Informatics and Terminology.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] Available from International Organization for Standardization (ISO), ISO Central Secretariat, BIBC II, Chemin de Blandonnet 8, CP 401, 1214 Vernier, Geneva, Switzerland, http://www.iso.org.

[4] Available from Committee on Data (CODATA) International Science Council, 5 rue Auguste Vacquerie, 75016 Paris, France, https://www.codata.org/nanomaterials.

3. Terminology

3.1 *Definitions*—For definitions of general terms used in this document, see *ASTM Online Terminology Dictionary of Engineering Science and Technology*.[5]

3.2 *Data Description Definitions:*

3.2.1 *descriptor, n*—numerical data or text that expresses the measurement, observation, or calculational result of some aspect of an object.

3.2.1.1 *Discussion*—A descriptor conveys both the semantics of the results as well as the result itself.

3.2.2 *information category, n*—a set or group of related descriptors that represent a property, characteristic, interaction, performance, or other feature of an object.

3.2.2.1 *Discussion*—Information categories may be hierarchical and contain subcategories (referred to as such), each containing a set of descriptors.

3.2.2.2 *Discussion*—Information categories and their subcategories are constructed to convey understanding of the structure, properties, features, and performance of an object.

3.2.2.3 *Discussion*—A descriptor may occur in more than one information category.

3.2.2.4 *Discussion*—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.

3.3 *Nanomaterials Terminology:*

3.3.1 *chemical moiety, n*—an identifiable part of a molecule that can act as a unit in chemical reactions.

3.3.1.1 *Discussion*—A moiety does not have to be able to exist separate from its inclusion in a molecule.

3.3.1.2 *Discussion*—A functional group is an example of a moiety, for example, the –COOH organic acid functional group.

3.3.2 *engineered nanomaterial, n*—nanomaterial designed for specific purpose or function.

ISO/TS 80004-1:2015(en), 2.8

3.3.3 *equivalency, n*—the ability of a description system to establish that two objects as assessed by different disciplines or user communities are the same according to specified criteria.

3.3.3.1 *Discussion*—In this guide, equivalency is the ability to establish that two nano-objects are the same according to specified criteria.

3.3.4 *manufactured nanomaterial, n*—nanomaterial intentionally produced to have selected properties or composition.

ISO/TS 80004-1:2015(en), 2.9

3.3.4.1 *Discussion*—Intentionally produced includes chemical, mechanical, electrical, nuclear, and other activities planned or controlled by humans.

3.3.5 *nanomaterial, n*—material with any external dimension in the nanoscale or having internal structure or surface structure in the nanoscale. **ISO/TS 80004-1:2015(en), 2.4**

3.3.6 *nano-object, n*—discrete piece of material with one, two or three external dimensions in the nanoscale.

ISO/TS 80004-1:2015(en), 2.10

3.3.6.1 *Discussion*—The second and third external dimensions are orthogonal to the first dimension and to each other.

ISO/TS 80004-1:2015(en), 2.5

3.3.6.2 *Discussion*—A nano-object is the smallest unit of nanomaterial that exists as a separate functional entity.

3.3.6.3 *Discussion*—A multilayer structure that is the smallest unit of nanomaterial with a specific functionality is defined herein to be a nano-object (see 3.3.5).

3.3.7 *nano-object feature, n*—a distinctive aspect of a nano-object.

3.3.7.1 *Discussion*—A nano-object feature can occur anywhere within or upon the nano-object.

3.3.7.2 *Discussion*—Within this guide, the term *nano-object feature* is sometimes referred to simply as a *feature*.

3.3.8 *naturally-occurring nanomaterial, n*—a nanomaterial made exclusively by natural processes.

3.3.8.1 *Discussion*—A naturally-occurring nanomaterial, when altered in any way by a process planned or controlled by humans, is, by definition, an engineered or manufactured nanomaterial.

3.3.8.2 *Discussion*—A nanomaterial produced by a natural process not planned or controlled by humans, for example, digestion or weathering of a rock, is naturally-occurring.

3.3.8.3 *Discussion*—There are instances when it is ambiguous or difficult to say whether a nanomaterial is naturally-occurring, engineered, or manufactured.

3.3.9 *uniquely, adv*—the quality of having uniqueness.

3.3.10 *uniqueness, n*—the ability of a description system to differentiate one nano-object from every other nano-object and to establish which specific nano-object is being described within the broad range of disciplines and user communities.

3.4 *Shape Terminology:*

3.4.1 *aspect ratio, n*—ratio of the extremal orthogonal dimensions of a nano-object.

3.4.1.1 *Discussion*—The aspect ratio reflects the fiber- or rod-like nature of a nano-object.

3.4.1.2 *Discussion*—The aspect ratio is sometimes called the sharpness of a nano-object.

3.4.1.3 *Discussion*—Aspect ratio applies to both two-dimensional and three-dimensional nano-objects.

3.4.2 *flatness, n*—ratio of the largest to smallest thickness for a two-dimensional-shaped nano-object.

3.4.2.1 *Discussion*—Flatness is sometimes referred to as thickness uniformity.

3.4.2.2 *Discussion*—This concept applies to both planar and non-planar shapes.

3.4.2.3 *Discussion*—See Fig. 3 and Fig. 4.

3.4.3 *sphericity, n*—ratio of the radii drawn from the geometric center of a nano-object to the closest and furthest surface features.

3.4.3.1 *Discussion*—Sphericity reflects how close a nano-object is to an ideal sphere; the closer the value is to 1, the more spherical is the nano-object.

[5] *ASTM Online Terminology Dictionary of Engineering Science and Technology*, available from ASTM International, ASTM Stock Number: DEFONLINE.

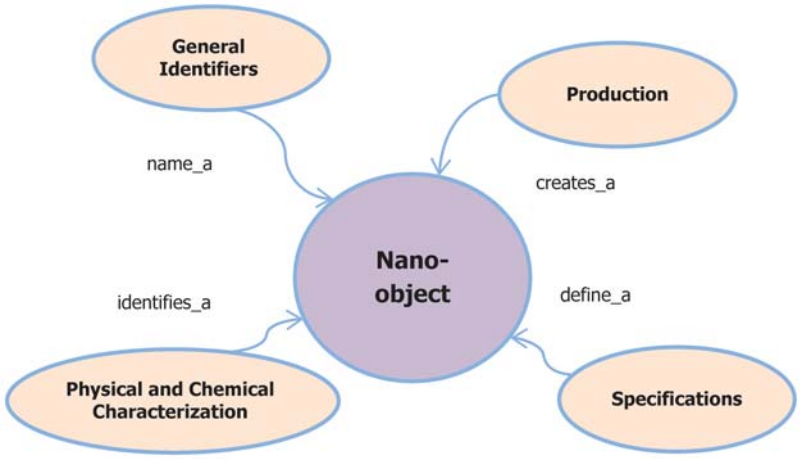

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FIG. 1 Data and Information Components Necessary to Describe a Nano-Object

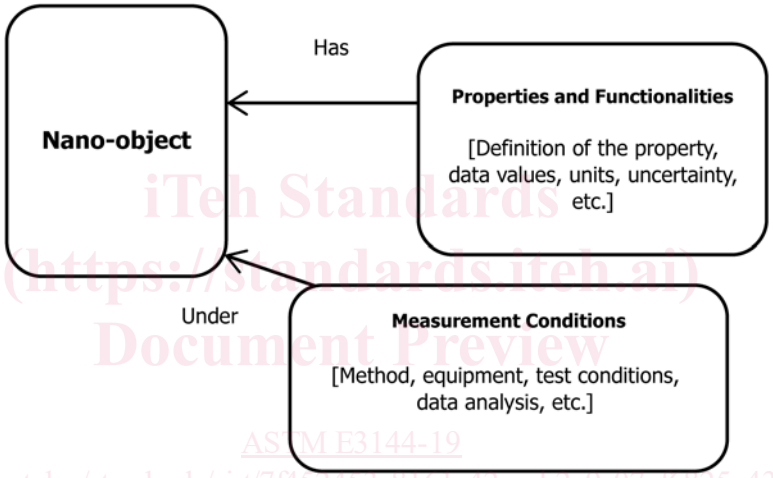

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FIG. 2 Data and Information Components Necessary to Describe a Nano-Object and its Properties

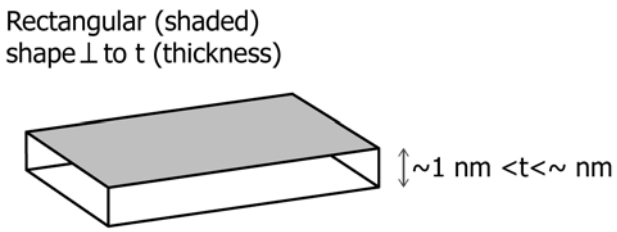

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FIG. 3 Geometrical Shape of a Nano-Object with One Dimension at the Nanoscale

3.5 *Size Terminology:*

3.5.1 *aerodynamic diameter, n*—diameter of a sphere 1 g cm-3 with the same terminal velocity in calm air as the particle, under the prevailing conditions of temperature, pressure, and relative humidity. **ISO 18158:2016 (en), 2.1.4.8**

3.5.1.1 *Discussion*—The particle aerodynamic diameter depends on the size, density, and shape of the particle.

3.5.2 *hydrodynamic diameter, n*—the diameter of a hard sphere that has the same diffusion behavior of the nano-object being measured.

3.5.2.1 *Discussion*—In purely geometric terms, the hydrodynamic diameter may be considered the volume-equivalent diameter.

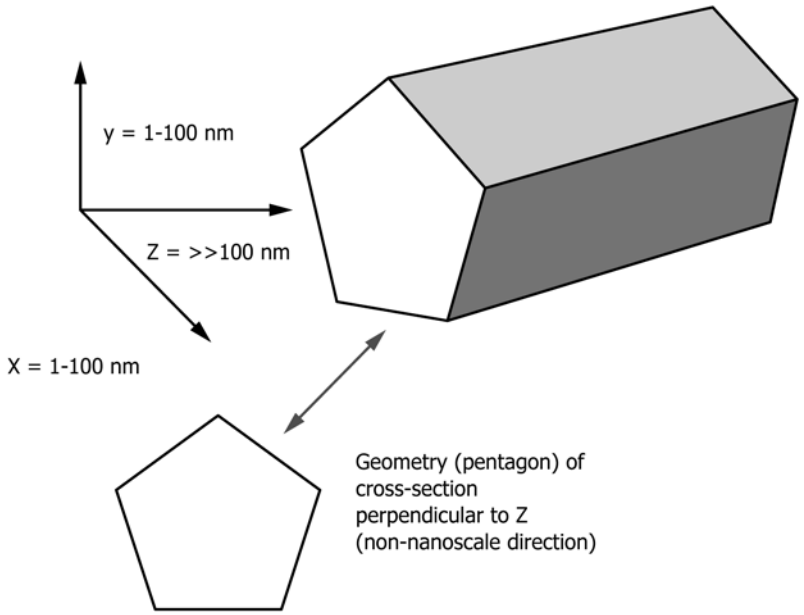

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FIG. 4 Geometrical Cross-Sectional Shape of a Nano-Object with Two Dimensions at the Nano-Scale

3.6 *Physical Structure Terminology:*

3.6.1 *adherent, n*—an object, such as a molecule, atom, biomolecule, polymer, nano-object, or other material in the nanoscale that is permanently or non-permanently attached to the surface of a nano-object in some manner.

3.6.2 *homogeneous physical structure, n*—a single phase nano-object that has uniform physical structure in any direction from the surface inward.

3.6.2.1 *Discussion*—Regardless of its shape, a homogeneous nano-object has the same chemical composition and crystallographic structure throughout.

3.6.3 *layer, n*—a two-dimensional structure of a nano-object with distinct edges whose third dimension is small with respect to the other two dimensions (Fig. 5).

3.6.4 *nanofibre (nanofiber), n*—a nano-object with two external dimensions in the nanoscale and the third dimension much larger. **ISO/TS 20787:2017(en), 3.12**

3.6.5 *nanoplate, n*—a nano-object with one external dimension in the nanoscale and the other two external dimensions significantly larger.

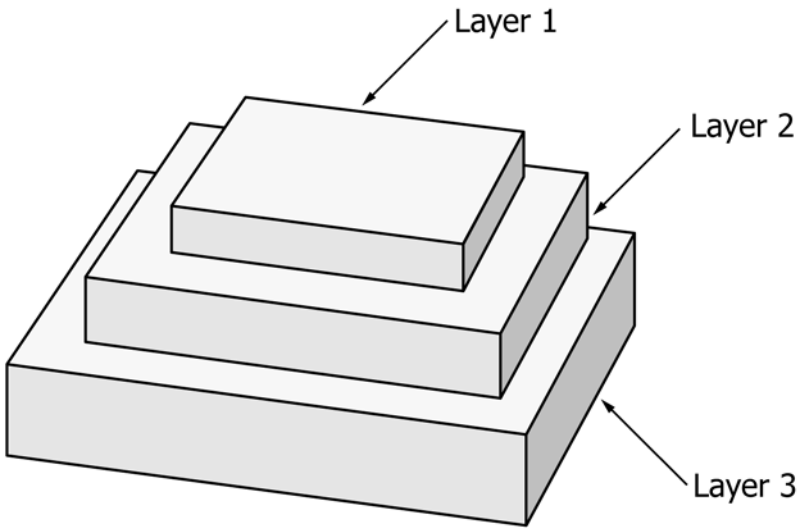

FIG. 5 Schematic Drawing of a Layered Nano-Object

3.6.5.1 *Discussion*—The larger external dimensions are not necessarily in the nanoscale.

3.6.6 *phase, n*—a bounded region of a nano-object with uniform chemical composition and crystallographic structure that can be mechanically separated from other regions of a nano-object.

3.6.7 *physical structure, n*—the physical arrangement of and relationship among the parts of a nano-object.

3.6.8 *shell, n*—a three-dimensional structure in a nano-object without distinct edges with one dimension (shell thickness) small with respect to the other two dimensions (Fig. 6).

4. Summary of Guide

4.1 This guide enumerates information categories and their contained descriptors used to report the physical and chemical characteristics of a nano-object. In practice, only a subset of information categories or descriptors will likely be used in each report instance.

4.2 Different amounts of data and information are generated in different measurement scenarios. For example, a researcher may concentrate on studying how shape influences the properties or functionalities of a nano-object. In this instance, the shape characteristics may be reported with more detailed information than for other characteristics.

4.3 Specification of a nano-object uniquely is critical in many applications.

4.3.1 For commercial transactions, specification of a nano-object uniquely ensures that a purchaser receives the desired product.

4.3.2 For research purposes, specification of a nano-object uniquely ensures that properties and functionalities can be correlated with true features of a nano-object as well as allowing others to duplicate research results.

4.3.3 For regulatory purposes, specification of a nano-object uniquely ensures that regulatory actions are applied only to the intended nano-object(s).

4.4 This guide can be used to determine that two nano-objects are the same with respect to their physical and chemical characteristics by comparison of the data reported using the information categories and descriptors defined herein.

NOTE 1—The choice of which information categories and descriptors to be compared is dependent on the application and context and is not defined in this guide.

4.5 When two or more nano-objects are specified uniquely and determined to be equivalent, data sets of their properties and functionalities may be combined on a scientifically valid basis to create larger data collections.

5. Significance and Use

5.1 A nano-object is an individual, well-defined, and separable piece of a nanomaterial; in practice, nanomaterials used in research, products, testing, and other uses are usually collections of nano-objects. Individual nano-objects and collections of nano-objects are the two major types of nanomaterials in use. The description of an individual nano-object is covered in this guide; the description of collections of nano-objects (for example, two or more individual nano-objects) is not covered in this guide.

5.2 Nanomaterials are of growing importance in research and commerce, and data on their physical and chemical characteristics are critical to predict performance, to transact commercial activities, to assess their potential for harm to human and animal health and the environment in general, and to support regulations that affect their use. To describe nanomaterials, whether for research or commerce, it is important to be able to describe an individual nano-object.

5.3 When in a liquid environment, a nano-object may attract a non-permanent "halo" of water or other solvent molecules; such a non-permanent halo is not described by the present guide.

5.4 In contrast, coatings and coronas are semi-permanent or permanent adherents on time scales commensurate with testing procedures; coatings and coronas can fundamentally transform one nano-object to another in terms of its characteristics and can be described using this guide.

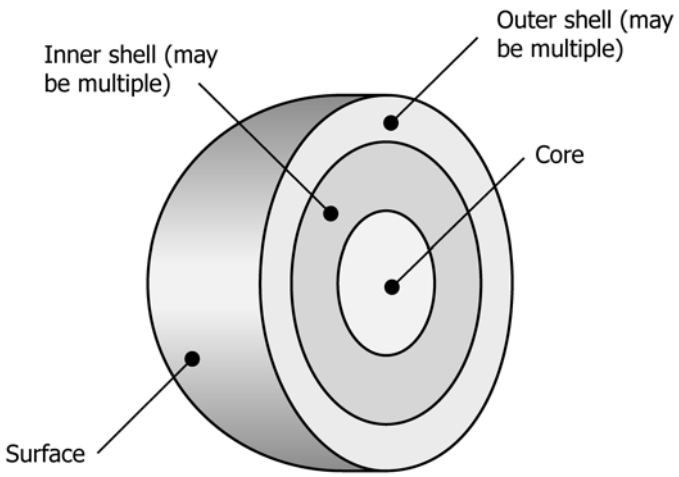

FIG. 6 Schematic Drawing of the Cross-Sectional View of a Nano-Object with a Shell-Like Structure

5.5 The four types of data and information used to describe a nano-object are: physical and chemical characteristics; production; specifications; and general identifiers (names and classifications), as shown in Fig. 1.

5.6 This guide deals solely with data and information to describe the physical and chemical characterization of an individual nano-object.

NOTE 2—Other guides and documents (see Section 2, Referenced Documents) deal with the data and information for production, specifications, and general identifiers (names and classifications).

NOTE 3—Specifications are formal or informal documents that provide guidance on specifying the composition, structure, or any other aspect of a nano-object.

5.7 In a practical sense, the amount of data and information reported to describe the physical and chemical characteristics differs widely depending on who is reporting and the reason they are reporting. Researchers examining specific aspects of a nano-object may choose to report a limited subset of characteristics. A test report on the potential toxicity of a nano-object may choose to report numerous characteristics. This guide supports both limited and complete reporting of the characteristics enumerated herein.

5.8 The science of characterizing nano-objects is still evolving. Some information categories will require additional descriptors as new knowledge is developed. Some descriptors may become obsolete. Users should consult the latest guide for the most complete recommendations.

5.9 The technology for collecting, storing, analyzing, and disseminating scientific and technical data continues to evolve, and tools such as ontologies, database schemas, data repository reporting requirements, and data recoding formats are evolving similarly. This guide provides a clear, English language definition of information categories and descriptors used to describe an individual nano-object that can be used in these and other similar tools.

5.10 A nano-object has properties and functionalities that are measured under specific measurement conditions. The description of a nano-object requires data and information on its properties as well as on the conditions under which those properties were measured, as shown in Fig. 2. The description of the data and information necessary to describe properties and functionalities as well as the procedure, which specify the measurement conditions under which the properties and functionalities are measured, are described in other guides and standards.

5.11 The characteristics of an individual nano-object defined in this guide address the important physical and chemical properties of that nano-object. Because the techniques and instruments used to measure these properties can greatly influence the property value, when available, the measurement result being used should include as much information as possible about the measurement conditions.

6. Information Categories and Descriptors

6.1 The six information categories, as given in Table 1, comprise characteristics of an individual nano-object relevant for its description that are covered in this guide.

TABLE 1 Information Categories for Describing the Physical and Chemical Characteristics (Intrinsic Properties) of a Nano-Object

Shape
Size
Physical structure
Chemical composition
Crystallographic structure
Surface description

NOTE 4—Other characteristics, not covered herein, may be useful in some circumstances.

6.1.1 Each of these information categories has several descriptors that provide quantitative and qualitative data for the characteristics of a nano-object.

6.1.2 While most descriptors to characterize a nano-object use data from measurement results using well-defined methods, other descriptors are more qualitative. As new methods for measuring the characteristics of nano-objects evolve, these qualitative descriptors will be replaced by quantitative ones.

6.2 *Shape:*

6.2.1 Characterization of the geometrical shape of a nano-object is critical as its properties and reactivity are strongly dependent on this factor. The descriptors required to describe quantitatively the shape of a nano-object are given in Table 2.[6]

6.2.2 Standard definitions have been established for many forms. The most common criterion for defining the shape of a nano-object is its general three-dimensional geometry, or shape type.

6.2.3 For shapes with external features, descriptors enumerate and describe those features.

6.2.4 Quantitative measures of shape include *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 provides an indication of how close a nano-object approaches the shape of a perfect sphere.

6.3 *Size:*

6.3.1 The modifier "nano" illustrates the importance of size in describing a nano-object, yet size even in the nanoscale can vary greatly. For example, the volume 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 the surface area of a 1 nm-sided cube. As many properties of nano-objects are surface area dependent, clearly size is important.

6.3.2 The size of features of a nano-object is also important and can also be reported. These features can be large-scale features that define the shape, such as the points of a star, or small-scale features, such as irregularities of a surface or large-scale feature.

6.3.3 In addition to overall size and the size of features, derived dimensions such as aerodynamic and hydrodynamic diameters can be reported.

[6] The boldface numbers in parentheses refer to a list of references at the end of this standard.