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Nanotechnologies — Model taxonomic framework for use in developing vocabularies — Core concepts

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National foreword

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Nanotechnologies — Model taxonomic framework for use in developing vocabularies — Core concepts

Nanotechnologies — Modèle de cadre taxinomique pour utilisation dans le développement de vocabulaires — Concepts de base



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Foreword

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In exceptional circumstances, when a technical committee has collected data of a different kind from that which is normally published as an International Standard ("state of the art", for example), it may decide by a simple majority vote of its participating members to publish a Technical Report. A Technical Report is entirely informative in nature and does not have to be reviewed until the data it provides are considered to be no longer valid or useful.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO/TR 12802 was prepared jointly by Technical Committee ISO/TC 229, *Nanotechnologies*, and Technical Committee IEC/TC 113, *Nanotechnology standardization for electrical and electronic products and systems*. The draft was circulated for voting to the national bodies of both ISO and IEC.

Other vocabulary documents developed by ISO/TC 229 and IEC/TC 113 include the ISO/IEC 80004 series, which consists of the following parts, under the general title *Nanotechnologies* — *Vocabulary*:

- ISO/TS 80004-1, Nanotechnologies Vocabulary Part 1: Core terms
- ISO/TS 80004-3, Nanotechnologies Vocabulary Part 3: Carbon nano-objects

The following parts are under preparation:

- ISO/TS 80004-4, Nanotechnologies Vocabulary Part 4: Nanostructured materials
- ISO/TS 80004-5, Nanotechnologies Vocabulary Part 5: Bio/nano interface
- ISO/TS 80004-6, Nanotechnologies Vocabulary Part 6: Nanoscale measurement and instrumentation
- ISO/TS 80004-7, Nanotechnologies Vocabulary Part 7: Medical, health and personal care applications
- ISO/TS 80004-8, Nanotechnologies Vocabulary Part 8: Nanomanufacturing processes

ISO/TS 27687:2008, Nanotechnologies — Terminology and definitions for nano-objects — Nanoparticle, nanofibre and nanoplate will be revised as ISO/TS 80004-2, Nanotechnologies — Vocabulary — Part 2: Nano-objects: Nanoparticle, nanofibre and nanoplate.

Introduction

This Technical Report provides a possible model taxonomic framework of core concepts for nanotechnology. The framework identifies the basic categories of nanotechnology, as well as the core concepts within these categories, and displays them in a hierarchical structure. From the core concepts, a list of core terms to be defined has been identified. Definitions for these terms will be developed in ISO/TS 80004-1, Nanotechnologies — Vocabulary — Part 1: Core terms. Definitions for terms in subject-related areas will be developed in other ISO/IEC Technical Specifications in the ISO/TS 80004 vocabulary series. See list in the Foreword

Communication is crucial to scientific practitioners, industry and trade, and regulatory bodies. Due to different backgrounds and needs, there can be widely divergent understandings and assumptions about concepts. The result is poor communication, a lack of interoperability among systems, and duplication of effort as different groups strive to define concepts in accordance with their perspectives.

A taxonomic framework of core terms is intended to place nanotechnology concepts into context by indicating relationships among these concepts. Such context can provide users with a structured view of nanotechnology and facilitates common understanding of nanotechnology concepts. Jointly, the model framework together with the core term definitions will be beneficial to industry, consumers, governments, and regulatory bodies because they promote clear, accurate and useful communication. Because the taxonomic framework looks at nanotechnology from a number of different viewpoints, it will minimize duplication of effort among stakeholders and assist in developing a harmonized vocabulary of terms.

This Technical Report attempts to remain current with the present usage of terms in this Technical Report and with the ongoing work by ISO/TC 229 and IEC/TC 113 to define such terms. However, definitions within the field of nanotechnologies are still evolving. Updating of this framework model for core concepts in concurrence with development of ISO/IEC vocabulary for nanotechnologies is recommended.

Nanotechnologies — Model taxonomic framework for use in developing vocabularies — Core concepts

1 Scope

This Technical Report establishes core concepts for nanotechnology in a model taxonomic framework. It is intended to facilitate communication and promote common understanding.

2 Purpose of the framework development

Taxonomy is a hierarchical classification of the things in a subject domain. It places the domain's concepts into relevant categories and shows the relationships among concepts. A core concept is one of the central concepts that define a subject domain. In taxonomy, these concepts are found at the topmost levels of the hierarchy.

A taxonomic framework for core nanotechnology concepts would have several purposes. As a representation of the professional judgment of an international group of scientists, it is a depiction of current understanding of the subject, its structure and relationships. It is considered to be a snapshot of the subject domain at a particular time and is intended to be revisited and updated as the domain develops. As well, because it deals only with the top layers of the nanotechnology hierarchy, it is considered to be a model framework from which development of deeper layers in the hierarchy should begin. Finally, this framework can be used as the basis for the development of terms and definitions for nanotechnology vocabulary.

3 Methodology

A library science approach is taken to create the taxonomy using ANSI/NISO Z39.19-2005 [1] and ISO 2788:1986 [2] as its foundation. Key concepts are categorized and, where possible, placed into hierarchical structures illustrated as framework diagrams in Clause 4, Framework development. Where a hierarchy could not be created a framework is presented as a basis for future hierarchy development.

The following steps created the core concept framework diagrams:

- Development of lists of concepts considered to be central to nanotechnology.
- Completion of a categorization exercise in which concepts were sorted in accordance with their similarities and differences.
- Building of hierarchical diagrams.

Framework and hierarchy illustrations are found in Clause 4, Framework development. For project methodology steps see Annex A.

Principles followed to ensure consistency:

— Things occurring naturally in the nanoscale are not addressed in this report.

- Certain terms under consideration have a common or established definition that renders them inappropriate to include in a core concepts framework specific for nanotechnology. For example in the "properties" framework development, it is necessary to include common terms to place terms specific to nanotechnology into their proper contexts.
- The term "nanoscale" is fundamental to nanotechnology and nanoscience and is a term defined in ISO/TS 27687:2008 [3], definition 2.1.

4 Framework development

The frameworks and hierarchies presented here provide starting points to support and guide the development of vocabulary for nanotechnologies. The frameworks are provided with the intention that they are to be altered and/or expanded on a hierarchical basis based on further expert input as knowledge and understanding evolves.

4.1 Fields of activity at the nanoscale

4.1.1 Diagram

The Fields of activity at the nanoscale framework diagram is shown in Figure 1. In this diagram the term "nanoscale" overarches nanotechnology and nanoscience.

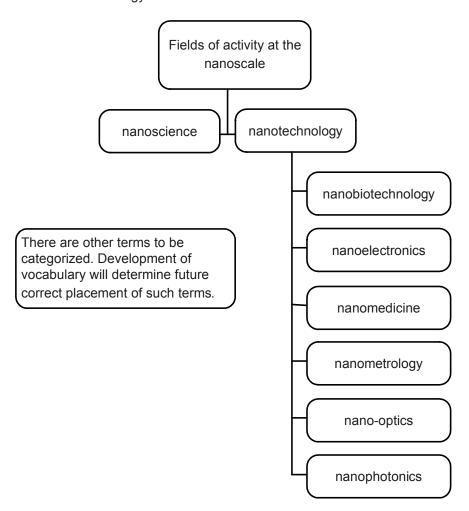


Figure 1 — Fields of activity at the nanoscale framework diagram

4.1.2 Discussion

The terms "nanoscience" and "nanotechnology" are indicated as equivalent hierarchy-level terms. The Figure 1 framework diagram is recommended to be additionally populated in subsequent editions, based on vocabulary developed in ISO/IEC Technical Specifications, *Nanotechnology* — *Vocabulary* (see list in the Foreword).

4.1.3 Advantages and disadvantages of the Fields of activity at the nanoscale framework

Arranging higher level concepts provides a short list of concepts that already have broad usage in literature and highlights a distinction between the scientific study of nanomaterials and the range of technological endeavours. The list of technologies provided is meant to be illustrative, not exhaustive, and should not be misinterpreted as excluding other legitimate areas that can be considered as being within the domain of nanotechnology.

4.2 Nanomaterial

4.2.1 Diagram

The Nanomaterials framework diagram is shown in Figure 2.

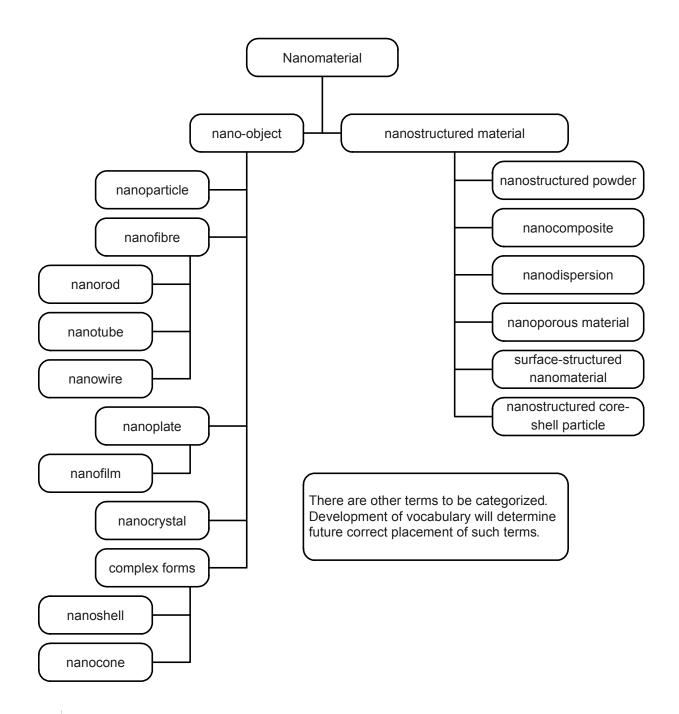


Figure 2 — Nanomaterial framework diagram

4.2.2 Discussion of the nano-object branch of the nanomaterials framework

This branch of the framework is developed as a hierarchy. The concept "ultrafine particle" is omitted from the hierarchy, consistent with ISO/TS 27687:2008 [3], A.3.2, Note, "Most nanoparticles, defined by their geometrical dimensions, are ultrafine particles, when measured". In addition:

- The concept "nanofibre" is the overarching concept that includes "nanorod", "nanotube", and "nanowire" ISO/TS 27687:2008 [3], Figure 2.
- Several concepts ("nanofilm" under "nanoplate", "nanocrystal", "nanoshell" and "nanocone" under "complex forms") are placed under different subsections and levels pending future revision in this framework based on terminology and definitions developed in ISO/IEC Technical Specifications, Nanotechnology Vocabulary (see list in the Foreword).

— "Carbon nanotube" is a concept that would be found deeper in the hierarchy under "nanotube". Carbon-based nano-objects are the subject of ISO/TS 80004-3, Nanotechnology — Vocabulary — Part 3: Carbon nano-objects.

4.2.3 Discussion of the nanostructured material branch of the nanomaterials framework

This branch is not developed as a hierarchy. The further development of core concepts for this branch remains under consideration during development of Technical Specification ISO/TS 80004-4, Nanotechnology — Vocabulary — Part 4: Nanostructured materials.

4.2.4 Advantages and disadvantages of the nanomaterials framework

The primary utility of the nanomaterials framework is to identify concepts and terms whose definitions will help in properly categorizing the subject domain. For some, nanocrystalline means having a crystalline structure, which may be in the shape of a nanoparticle, nanofibre or nanoplate. For others, it is part of a larger object, but one that might place it in the nanostructured material category. The inclusion of a "complex forms" sub-branch implies that just particle, fibre, and plate categories are insufficient. The "complex forms" sub-branch may need to be further populated, and concepts re-visited and placed accordingly when terminology and definitions are further developed in ISO/IEC Technical Specifications, *Nanotechnology* — *Vocabulary* (see list in the Foreword).

4.3 Processes

4.3.1 Diagram

The Processes framework diagram is shown in Figure 3.

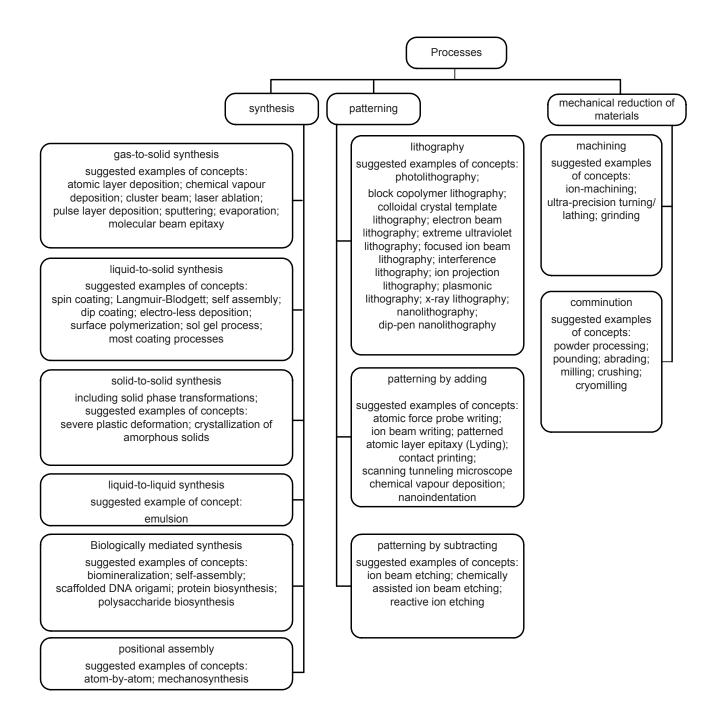


Figure 3 — Processes framework diagram

4.3.2 Discussion

This framework is partially developed as a hierarchy. Specifically, a hierarchy is not imposed beyond the three major headings, synthesis, patterning, and mechanical reduction of materials. The examples are appropriate for the sub-headings and are suggested to be further populated when terminology and definitions are further developed in ISO/IEC Technical Specifications, *Nanotechnology* — *Vocabulary* (see list in the Foreword).

Expanded expertise and development in ISO/TS 80004-8, Nanotechnologies — Vocabulary — Part 8: Nanomanufacturing processes may further expand this hierarchy. This framework evolved through several

different structural forms, as well as a name change from "Nanomanufacturing processes" to "Processes" 1). The core concepts "top-down nanomanufacturing" and "bottom-up nanomanufacturing" are not included. These concepts have limited value in the hierarchy shown in Figure 3 as some processes do fit neatly into bottom-up and top-down categories while others such as nanopatterning can be done using both bottom-up and top-down processes.

The framework uses three major subtopics: "synthesis" (the creation of the object); "patterning" (the process by which the surface of a pre-existing substrate is altered to create nanoscale features); and "mechanical reduction of materials" (the processes by which a large object is reduced in size to become a nanoscale object). Biologically-mediated processes are viewed as belonging in the "synthesis" branch.

The "synthesis" branch underwent significant changes before reaching the state depicted in Figure 3. Initially, this branch utilized the traditional disciplines of chemistry, physics and biology as the three major subtopics for synthesis. (This earlier version of the "synthesis" branch is included for information in Annex B.) The earlier organization of concepts proved problematic. Several sub-terms, such as "deposition", appeared repeatedly, reflecting the overlap that exists between chemistry and physics. Synthesis as a process is considered to encompass reactants undergoing:

- a) a change in molecular structure;
- b) a change in state (gas, liquid, solid); or
- c) a change in phase (emulsification or change in crystallinity) to form a nano-object.

In the "mechanical reduction of materials" branch, machining refers to the deliberate removal of material through operations such as drilling, lathing, milling (cutting) or burnishing, normally accomplished mechanically in a machine shop using machine tools. This subcategory comes closest to the concept "top down", where machining involves nanoscale control. Comminution involves grinding, impact erosion and other operations that alter shape as well as size.

4.3.3 Advantages and disadvantages of the processes framework

The framework distinguishes patterning and the creation of patterns from synthesis and mechanical reduction of materials. This distinction is important as it is the basis for much of today's semiconductor industry. Additionally, the diagram identifies where the concept of engineered nanomaterials overlaps the most with naturally occurring ultrafine materials of use to industry. Naturally occurring materials would most likely be mined, purified and sized by the processes found under "mechanical reduction of materials", while the designed generation of newer substances would be found under "synthesis". This can be considered in the development of terminology and definitions for nanomanufacturing processes.

4.4 Nanosystems and nanodevices

4.4.1 Diagram

The Nanosystems and nanodevices framework diagram is shown in Figure 4.

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¹⁾ This name change is necessary because the broad nature of the first level concepts of the hierarchy failed the all-and-some test when "Nanomanufacturing processes" is the main heading. The first level concepts in the current hierarchy in Figure 3 demonstrate how the all-and-some test failed. The test proved the following statements to be untrue: Some nanomanufacturing processes are synthesis; all synthesis is a nanomanufacturing process. (Synthesis is not exclusively a *nanomanufacturing* process.) See Annex B for more information about the all-and-some test.

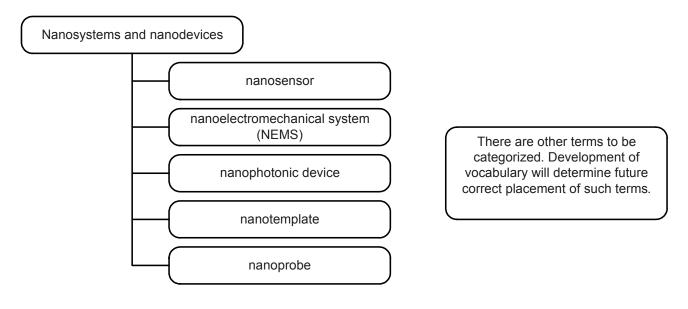


Figure 4 — Nanosystems and nanodevices framework diagram

4.4.2 Discussion

This framework is not developed as a hierarchy. Nanosystems and nanodevices are core concepts in the medicine, biology, electronics and information technology fields. Terminology and definitions developed in ISO/IEC Technical Specifications, *Nanotechnology* — *Vocabulary* (see list in the Foreword) may allow further development of this framework.

4.5 Properties

4.5.1 General

Creation of a single framework illustrating the properties, states and/or phenomena relating to nanomaterials presents complexity in placing these multiple concepts in diagram form. Therefore four versions of properties frameworks are presented. Future review on how they can be used, developed or discarded is recommended in conjunction with the development of terminology and definitions for nanotechnologies in ISO/IEC Technical Specifications, *Nanotechnology — Vocabulary* (see list in the Foreword).

A nano-effect may be defined as an abrupt change in magnitude (value) occurring within the nanoscale of 1 nm to 100 nm or may be a significant change in magnitude (value) when referenced to a macroscale sample of the same material. Phenomena and properties at the nanoscale are known and well established scientifically at the macroscale such that there are no "unique" properties observed solely at the nanoscale and no "unique" materials (a material present solely at the nanoscale). There remains the possibility for distinct combinations of properties to exist for a given material at the nanoscale that in turn offers opportunities for novel uses and applications. In such cases, an eventual, unified understanding of such phenomena will come from continued research.

A change in magnitude (value) for a property is a possibility as a material's dimensions move from the macroscale to the nanoscale. One difficulty for scientists is to decide if the reference frame for comparison should be a length (dimension), as given in ISO/TS 27687:2008 [3], or the surface area, or the volume, concepts that unfortunately are all included in the English term, "bulk". This difficulty is also present when attempting to provide a visual representation on how properties, phenomena and states are associated with each other.

Duplicate entries, questions about hierarchy, and the limits of language occurred for each visualization. As a simple example, adsorption phenomena should be related to surface area and also the curvature of the surface (convex or concave), which relates to length for a nanoparticle but not for a nanofibre. Considerations such as these are subjects for future review.

4.5.2 Version 1 properties framework

4.5.2.1 Diagram

Version 1 of a Properties framework diagram is shown in Figure 5. This version uses the category outlined in ANSI/NISO Z39.19 [1] ("Properties or states of persons, things, materials and actions"). It attempts to classify properties related to nanotechnology in general, rather than to nanomaterials specifically.

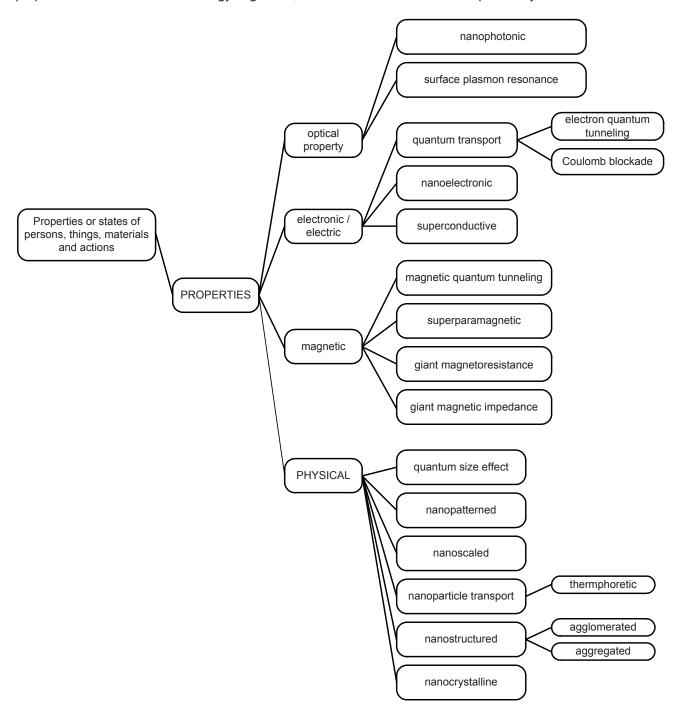


Figure 5 — Version 1 properties framework diagram

4.5.2.2 Advantages and disadvantages of version 1 properties framework

The framework highlights that collective properties may be central to identifying those phenomena most likely to be distinctive at the nanoscale. However the framework does not satisfactorily address mechanical properties. Moreover, physical properties encompassed virtually all the properties listed.

4.5.3 Version 2 properties framework

4.5.3.1 Diagram

Version 2 of a properties framework diagram is shown in Figure 6. Version 2, like version 1, uses the category outlined in ANSI/NISO Z39.19 [1] ("Properties or states of persons, things, materials and actions"). It attempts to classify properties related to nanotechnology in general, rather than to nanomaterials specifically.

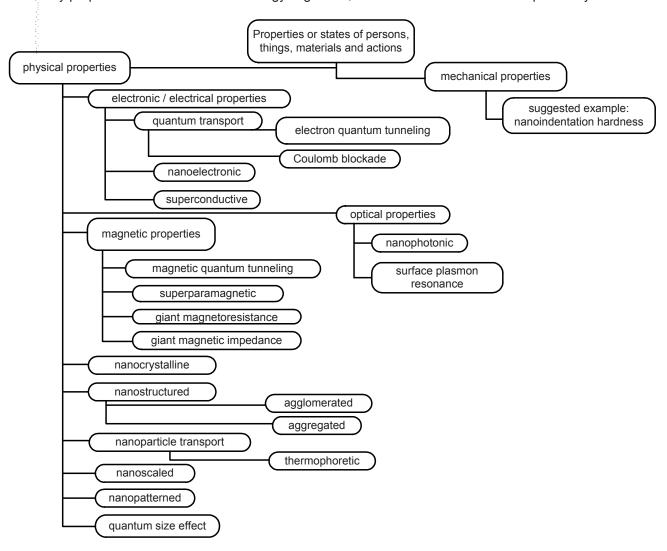


Figure 6 — Version 2 properties framework diagram

4.5.3.2 Advantages and disadvantages of the version 2 properties framework

This version does not encompass aspects of nanotechnology involving collective properties or those systems where current knowledge is based on the phenomena observed without certainty as to the properties associated with that phenomenon (e.g. interactions among nanomaterials; toxicology).

4.5.4 Version 3 properties framework

4.5.4.1 Diagram

Version 3 of a properties framework diagram is shown in Figure 7. The main title of the diagram is changed to "Properties/states/phenomena relating to nanomaterials". This change reflects recognition that the concepts of "phenomena" and "nano-effect" needed to be included in this framework and that the focus of the framework should be on nanomaterials specifically, as opposed to nanotechnology in general.

Most concepts in Figure 7 under the properties and phenomena headings are not specific to nanotechnology but have relevance in making, characterizing and using nanomaterials.

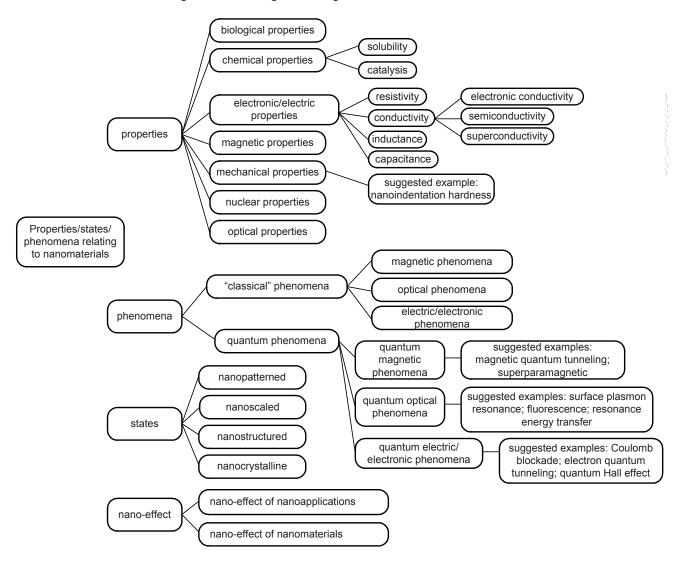


Figure 7 — Version 3 properties framework diagram

4.5.4.2 Advantages and disadvantages of the version 3 properties framework

The questions surrounding science and technology come back in this framework. A science is traditionally based on the ability to describe phenomena and relate the magnitude of the observation to properties of materials. A state is often defined as a complete description of the system involved (e.g. a thermodynamic state). If the study of nanoscale systems is a science, then the ability to define the nano-state becomes necessary. If, on the other hand, the topic is solely a technology of manipulating materials, then nanoeffects will become the focal point. In either case, having a more comprehensive view of the observable effects

assignable to nanoscale materials is a necessary first step. Value is found in separating the concepts of properties and phenomena. The correspondence between each phenomenon and its associated properties should be developed. This framework does not highlight or isolate nano-specific effects.

In Figure 7, hierarchical relationships have not been established between the subtopics "properties", "phenomena", "states", and "nano-effect" and the main topic. Unanswered questions include whether the concept of "properties" subordinate to the concept of "phenomena" and whether a "nano-state", demonstrated by a material exhibiting a nano-effect, is observed with larger sizes of the same material. This led to the Version 4 properties framework in Figure 8 which is based on a comprehensive listing of properties exhibited by materials at the nanoscale from scientific literature.

4.5.5 Version 4 properties framework

4.5.5.1 Diagram

Version 4 of a properties framework diagram is shown in several parts due to its complexity. It is presented first in Figure 8 showing the main topic with five subtopic branches. Figures 9 to 13 show the branches for each subtopic in detail.

This framework focuses on factors in the subtopic branches that result in properties exhibited by materials at the nanoscale. These factors include particle size, specific surface area, surface curvature, macroscopic surfaces, or composite materials. Suggestions are given to the properties involved recognized to be pragmatic, measurable observations.

NOTE Factors indicated in subtopic branches may overlap or be linked for some nano-objects.

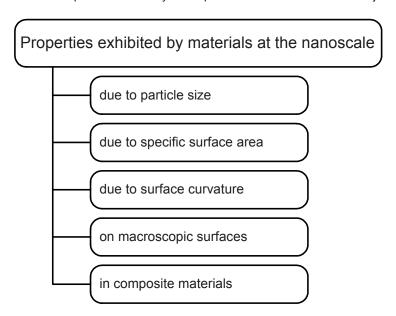


Figure 8 — Version 4 properties framework diagram with subtopic names

Figure 9 — Version 4 properties framework diagram - nanoscale properties due to particle size branch

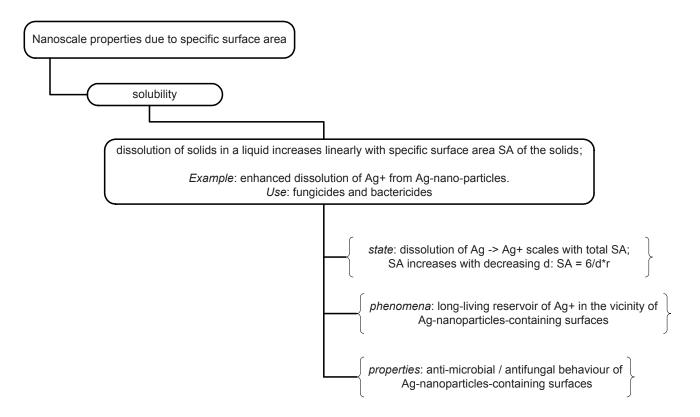


Figure 10 — Version 4 properties framework diagram – nanoscale properties due to specific surface area branch

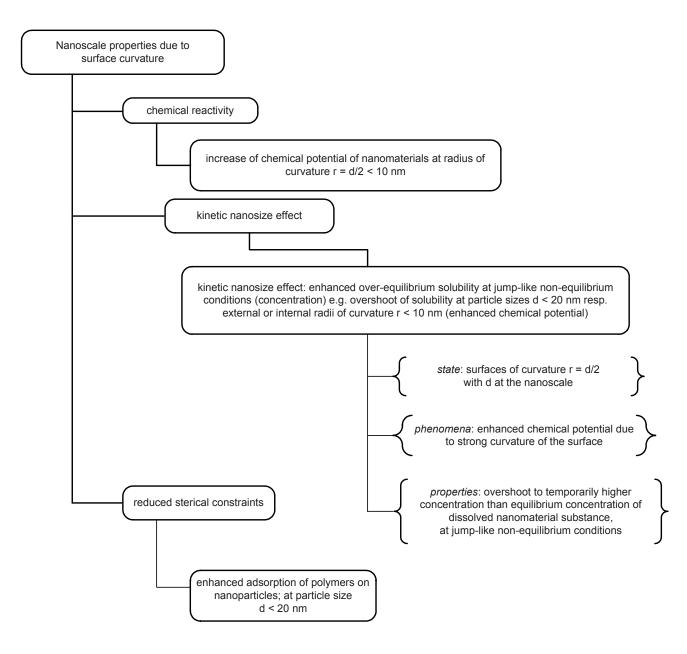


Figure 11 — Version 4 properties framework diagram – nanoscale properties due to surface curvature branch

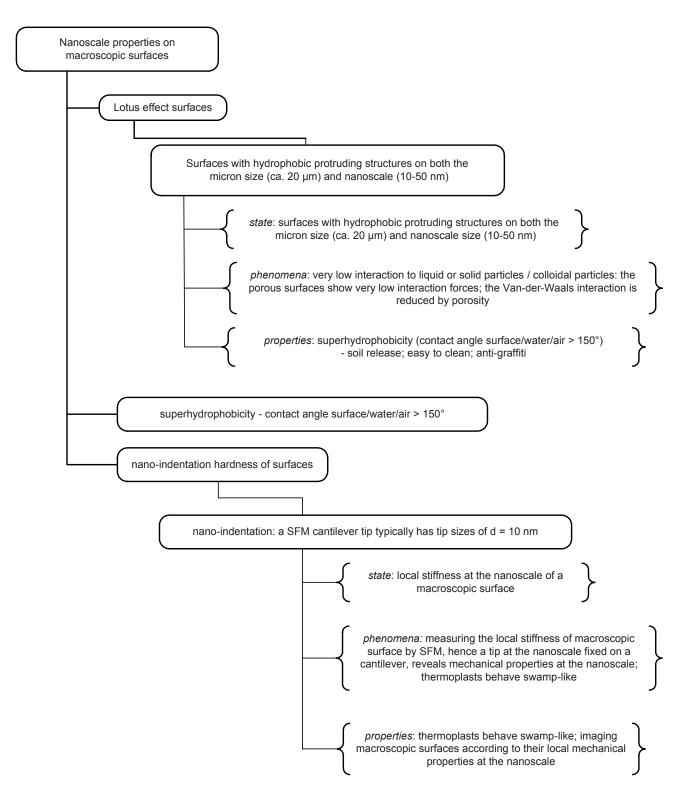


Figure 12 — Version 4 properties framework diagram – nanoscale properties on macroscopic surfaces

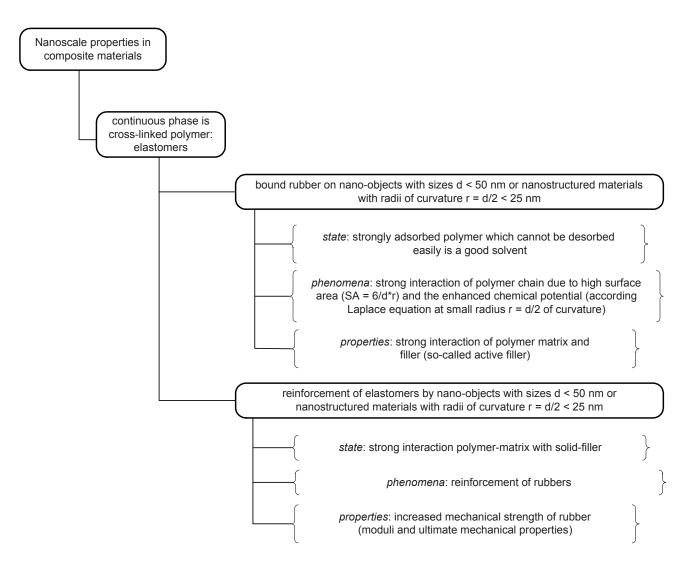


Figure 13 — Version 4 properties framework diagram – nanoscale properties of nanocomposite materials branch

4.5.5.2 Advantages and disadvantages of the version 4 properties framework

The advantage of this nanoscale properties viewpoint is that it can serve as a precursor to a future "properties, phenomena, states" visualization. It contains no assumptions about associating phenomena with specific properties or *vice versa*. One can plausibly argue that the dynamic state of nanotechnology is such that pragmatic observations will point to the later description using phenomena and properties, which in turn will lead to the development of a science.

This is a pragmatic approach that emphasizes technology rather than science in its structure. Further case studies will be needed to make the framework more comprehensive. An improved hierarchy may emerge from this effort.

Annex A

(informative)

Development steps for the core concept framework diagrams

Development steps for the core concept framework diagrams:

- a) Lists of concepts compiled central to nanotechnology, from an inventory of approximately 400 terms from nanotechnology-related presentations. The list is not considered to be exhaustive.
- b) Subsequent professional judgment generated a base list of 82 terms. While this list formed the basis of the following step in the methodology, terms were added and removed based on scientific judgment during development.
- c) A categorization exercise sorted concepts in accordance with their differences and similarities. Concepts could appear in one category only. This produces a series of flat lists of concepts within specific categories before the next steps that place concepts in hierarchical order.
- d) Categories reviewed as outlined in ANSI/NISO Z39.19-2005 ¹, pp. 23-24. The categories list, which is not exhaustive, includes the following:
 - 1) things and their physical parts;
 - 2) materials:
 - 3) activities or processes;
 - 4) events or occurrences;
 - 5) properties or states of persons, things, materials, or actions;
 - 6) disciplines or subject fields;
 - 7) units of measurement.
- e) Categories modified to suit the nanotechnology subject domain.

For example, there is little conceptual difference in the terms placed in the "Activities or processes" and "Events or occurrences" categories so this category becomes solely "Activities or processes", and then ultimately "Processes". "Articles and their physical parts" underwent several name changes settling on "Nanosystems and nanodevices". "Materials" changed to "Nanomaterial". "Disciplines" changed to "Fields of activity at the nanoscale". "Units of measurement" is not used.

The final list of categories is:

- 1) fields of activity at the nanoscale;
- 2) nanomaterial;
- 3) processes;
- 4) nanosystems and nanodevices;
- 5) properties.

The "properties" category developed under three headings:

Properties or states of persons, things, materials, or actions;

Properties/states/phenomena relating to nanomaterials; and,

Nanoeffects of nanomaterials

- f) Using the flat lists from the categorization exercise, hierarchies are built and tested for hierarchical soundness with tests as follows:
 - 1) The "is a" test, to verify the statement "a [narrower concept] is a [broader concept]". For example, a mammal *is a* vertebrate. This test identifies the link between a category and its members ANSI/NISO Z39.19-2005 [1], p. 47.
 - 2) The "all-and-some" test, which checks the logic of the hierarchy. In this test, one verifies the statements "Some [broader concepts] are [narrower concepts]. All [narrower concepts] are [broader concepts]". For example, the following statement passes the test: Some succulent plants are cacti. All cacti are succulent plants. However, the following statement fails the test: Some desert plants are cacti. Some cacti are desert plants. That is, some desert plants are cacti, but not all cacti are desert plants ANSI/NISO Z39.19-2005 [1], pp. 47-48.

Taxonomy can depict several kinds of relationships, including hierarchical, polyhierarchical, and associative relationships.

Hierarchical relationships include the following:

- I) Generic: an "is a" relationship: a personal digital assistant is a computer.
- II) Whole-part (partitive): an "is part of" relationship: Frankfurt is part of Germany; a lens is part of a camera.
- III) Instance: an "is a" relationship, showing specific examples which are frequently proper nouns: the Arctic Ocean is an ocean; the Alps are a mountain range. ANSI/NISO Z39.19-2005 [1], pp. 46-49.

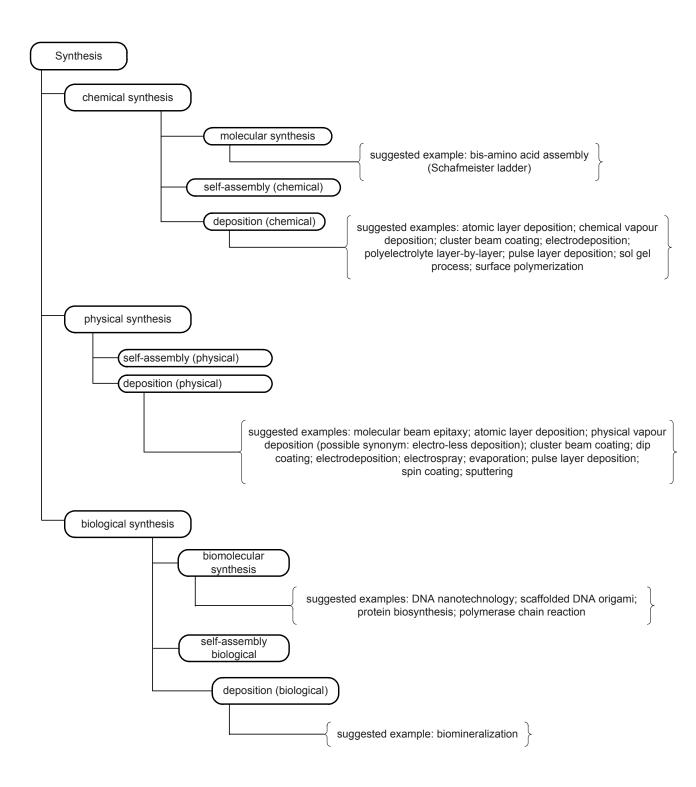
Polyhierarchical relationships show concepts as logically belonging to more than one category. For example, the concept "piano" belongs in both the "stringed instruments" and "percussion instruments" categories ANSI/NISO Z39.19-2005 [1], pp. 49-50.

Associative relationships are not hierarchical but show concepts as having a thematic or semantic relationship that should be mentioned in the taxonomy ANSI/NISO Z39.19-2005 [1], pp. 51-55. For example, the concept "shovel" can be associated with the concept "digging".

The development of frameworks for core concepts used hierarchical relationships only.

Annex B (informative)

Alternate version of the "synthesis" branch of the processes framework diagram



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- [4] ISO/TS 80004-1, Nanotechnologies Vocabulary Part 1: Core terms
- [5] ISO/TS 80004-3, Nanotechnologies Vocabulary Part 3: Carbon nano-objects
- [6] ISO/TS 80004-4, Nanotechnologies Vocabulary Part 4: Nanostructured materials
- [7] ISO/TS 80004-5, Nanotechnologies Vocabulary Part 5: Bio/nano interface
- [8] ISO/TS 80004-6, Nanotechnologies Vocabulary Part 6: Nanoscale measurement and instrumentation
- [9] ISO/TS 80004-7, Nanotechnologies Vocabulary Part 7: Medical, health and personal care applications
- [10] ISO/TS 80004-8, Nanotechnologies Vocabulary Part 8: Nanomanufacturing processes

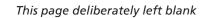
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²⁾ ISO/TS 27687:2008 will be revised as ISO/TS 80004-2, Nanotechnologies — Vocabulary — Part 2: Nano-objects: Nanoparticle, nanofibre and nanoplate.

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