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Towards the taxonomic categorization and recognition of nanoparticle shapes

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Abstract

The shape of nanoparticles and nanomaterials is a fundamental characteristic that has been shown to influence a number of their properties and effects, particularly for nanomedical applications. The information related with this feature of nanoparticles and nanomaterials is, therefore, crucial to exploit and foster in existing and future research in this area. We have found that descriptions of morphological and spatial properties are consistently reported in the nanotechnology literature, and in general, these morphological properties can be observed and measured using various microscopy techniques. In this paper, we outline a taxonomy of nanoparticle shapes constructed according to nanotechnologists' descriptions and formal geometric concepts that can be used to address the problem of nanomaterial categorization. We employ an image segmentation technique, belonging to the mathematical morphology field, which is capable of identifying shapes in images that can be used to (semi-) automatically annotate nanoparticle images.

From the Clinical Editor: This team of authors outlines a taxonomy of nanoparticle shapes constructed according to nanotechnologists' descriptions and formal geometric concepts enabling nanomaterial categorization. They also employ a mathematical morphology-based image segmentation system, capable of identifying shapes and can be utilized in semi-automated annotation of nanoparticle images.

Key words: Nanoparticle shapes; Taxonomic categorization; Nanoinformatics; Image processing; Watershed segmentation

Shape is a fundamental characteristic of components of living beings and entities such as viruses, cells, bacteria, organs, and, from an atomic perspective, of molecules and macromolecules, which includes nanoparticles. Regarding the latter, important characteristics of nanoparticles to medical applications such as drug delivery capabilities, adsorption, or the effectiveness of "nanodrugs" have shown to be influenced by the shape they present.[1–6]

A fundamental and pending problem in nanotechnology is the categorization and nomenclature of nanoparticles. To address this problem, two essential criteria have been identified[7]: uniqueness -so we can know exactly what materials we are talking about- and equivalence -to indicate if two materials are essentially the same one.

One of the first attempts for classifying nanostructured materials was made by Gleiter,[8] who considered the heterogeneousness of nanocompounds and the dimensionality of nanocomponents. This approach was extended by Pokropivny and Skorokhod,[9] combining the dimensionality of the nanocompounds. Similarly, Tomalia[10] proposed the development of a "periodic table" of nanoparticles and nanomaterials, including "shape" and "size" as two characteristics. Given the variability of these morphospatial characteristics of nanoparticles and nanomaterials,[11] knowing the shapes and forms of nanoparticles can be a necessary component of future classifications of nanoparticles and an aid in discerning mechanisms for their interactions in different environments.

The development of new nanomaterials by design requires categorizations of candidate materials based on their mechanisms of action. These mechanisms of action depend on a range of particle properties such as size, shape, crystal structure, reactivity, electronic band structure, toxicity, or affinity to biomolecules, etc., in addition to the properties of the media in which they are dispersed. Consequently, any categorization effort should accommodate annotation and mappings with respect to additional properties. Moreover, there is a growing need for the research

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community to label existing nanoparticles according to other properties beyond their physical, chemical, or structural information. For instance, the production technique employed in their manufacture or even their manufacturing lot number may be needed to correctly differentiate nanoparticles of the same type with respect to their purity, contaminants and lot-to-lot variability.

In this work, we propose an approach to manage these features of nanoparticles and nanomaterials by the use of a visual computational taxonomy. Ontologies have been shown to be a fundamental tool for scientific research in a large number of fields,[12] serving as a reference for knowledge management. Examples such as the Gene Ontology[13] are representative of such a trend. Current ontologies are based on textual information about the represented domains. Ontologies formally represent knowledge by structuring the semantics associated with the terms used in particular disciplines and/or use cases in a machine-interpretable way.[14] By gathering those terms, they generate a framework for terminology standardization.[15] However, this approach does not consider a fundamental aspect of many entities, such as living beings: their visual components and features. The representation of visual characteristics-such as shapes-has not been disregarded in current applied ontologies[16–18]; the Foundational Model of Anatomy,[17] to name an example, is an ontology designed to represent human anatomy. This ontology represents spatial information with textual descriptions, using terms such as “ventral”, “dorsal”, “axis”, etc. In this and other ontologies that must deal with a variety of shapes, their descriptions are usually qualitative. However, to establish spatial relationships between visual entities quantitatively it is necessary to incorporate different types of characteristics and information, which can rely, for instance, on mathematical theories of geometry, topology, and sets. In this context, geometry-based descriptions can provide a broad set of theories, methods, and tools to efficiently manage the visual information related to shapes. Shape and geometric classic ontologies have been applied to a number of different domains, such as bird classification,[19] engineering processes,[20,21] or imaging[22] and visual reasoning,[23] with limited success. Classical approaches to describe shapes through textual descriptions cannot deal efficiently with the graphical, visual information that shapes imply, typically losing the geometric formality inherent to shapes that could provide quantitative measures together with current laboratory instrumentation, measurement techniques, or computational methods.

While conceptual approaches for building taxonomies, ontologies, and classifications have contributed to facilitate the management of morphospatial information, they cannot replace the processing of visual and spatial information. In such a context, we propose an approach to build a taxonomic classification of nanoparticle and nanomaterial shapes based on quantitative measures of geometric features following recent developments in shape metrology.[24] Our approach bears in mind the future complementarity with other classification efforts.

Finally, the use of computational techniques to examine and extract visual features is frequently used in a wide range of fields. In addition to the visual taxonomy of nanoparticle shapes, we use an imaging technique developed at the Biomedical Informatics Group laboratory[25]: the Shape-Preserving Watershed (SPW); that can recognize shapes in nanoparticle images and facilitate their automatic annotation and categorization.

Methods

Extraction of common nanoparticle shape names

To develop an early version of a visual taxonomy of nanoparticle shapes, based on their morphological characteristics, we have based our work on morphological descriptions provided in the literature. We have preliminarily studied a selection of 35 nanotechnology papers that address topics such as the characterization of nanostructures or descriptions of nanocompounds. These papers were selected and used to make an initial listing of the terms used to describe shapes of nanometer sized elements such as nanoparticles and nanomaterials composites. In these papers, the most commonly used terms in 2D stem from the frequent description of benzene rings or graphene patterns (hexagon), the recurrent depiction of elliptical compounds and cells (ellipse, circle, plate), and the projections of crystals in the form of polygonal shapes (rectangle, square, triangle), to name a few. On the other hand, the use of 3D shape terms in the literature is more frequent -the number of appearances is almost four times higher-. The most used terms arise from the classical equilibrium shape of many chemical compounds (sphere), from helical structures, from toroids (rings), from classic arrangements of crystals (cube), and from cylindrical structures (column, wire, rod). Further details on the extraction of the shape terms used to describe nanometer scaled complexes can be seen in the Supplementary Information.

Taxonomic hierarchization of shapes

We have observed that shape terms used by nanotechnologists, in these and other papers, often lack the appropriate geometrical descriptions to directly create any formal taxonomy. To address this issue, we have elaborated a mapping of these terms to formal geometric classes, considering the following:

a) 2D and 3D shapes are the two main geometric subclasses in which shape terms from the literature can be classified;
b) For 2D classes the main subclass is “polygon” due to its importance for numerous geometric operations and applications. Depending on the number of sides, other subclasses will emerge (e.g., triangle, quadrilateral, pentagon…);
c) In 2D shapes, ellipses (and the particular case of the circle) are important, too, since many shapes of nanoparticles seem to show a natural elliptical shape;
d) For 3D shape class, the “polyhedron” subclass is the analogous case of 2D polygons. Depending on the number and the arrangement of their faces, a large set of polyhedrons may be derived; and
e) The third dimension makes available a broader set of shapes than the one provided by 2D forms. Thus, other important shapes, such as cones, cylinders, and toroids, can be considered as subgroups of 3D shapes.

We must note that this mapping implies the annotation of the synonyms of those less-formal shape terms. Thus, regarding the classic approach, sets of synonyms can be attached to the visual entities of shapes. For instance, the wire term corresponds to the Cylinder class in our taxonomy, which is represented as the surface that joins two parallel coaxial circles.