

Properties of Nanomaterials

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1 Introduction to Nanomaterials

Nanomaterials usually defined as materials composed of a set of substances where at least one dimension is less than approximately 100nm providing unique physical and chemical properties that exist at the nanoscale.

Because of the unique nanoscale (1–100nm) size, nanomaterials are different from microscopic atoms molecules and macro-objects in terms of their physical, chemical, electrical, and magnetic properties. The properties of macroscopic material abruptly change to some exceptional properties because of the size reduction. Nanocrystalline materials with very fine grain size show drastically different mechanical properties such as superplasticity, exceptional hardness toughness, and strength compared to conventional microstructures.

2 Physical Properties

2.1 Size and shape of nanomaterials

As per size and dimension, nanomaterials can be classified into four categories:

- (1) Zero-dimensional nanomaterials (0-D): All three dimensions confined to the nanoscale. Examples are **quantum dots, fullerenes, and nanoparticles**. However, cubic and polygonal shapes with nanodimensions are also found under this class. They can be amorphous, single crystal line, or polycrystalline.
- (2) One-dimensional nanomaterials (1-D): Two dimensions confined to nanoscale and one is extended in one dimension. Examples are **nanotubes, nanofibers, nanorods, nanowires, and nanohorns**. 1D nanomaterials offer unique advantageous properties due to their inherent high-aspect-ratio structural feature in conjunction with superior mechanical, electrical, and optical properties.
- (3) Two-dimensional nanomaterials (2-D): One dimension confined to nanoscale and other two are extended beyond. Examples are **nanosheets, nanofilms, and nanolayers**.
- (4) Three-dimensional nanomaterials (3-D) or bulk nanomaterials: There is no confinement to the nanoscale, meaning all the three dimensions are extended. Examples are **Nanoballs, Nanocones, Nanopillars and Nanoflowers**. 3D nanomaterials can contain dispersions of nanoparticles, bundles of nanowires, and nanotubes as well as multilayers. [2]

Let a material(i.e., 0D, 1D, 2D and 3D) is plotted with energy E on the X-axis and $g(E)$ (density of states) on the Y-axis and E_g is band gap energy. Look at Figure 1

2.2 Surface effects

Nanomaterials possess a large fraction of surface atom per unit volume. Thus nanomaterials possess high surface area over volume ratio, which leads them to interact with the environment more effectively compared to bulk materials. The surface-to-volume ratio scales with the inverse size, and therefore there are other properties such as phase transition temperature and solubility also obey the same scaling law.

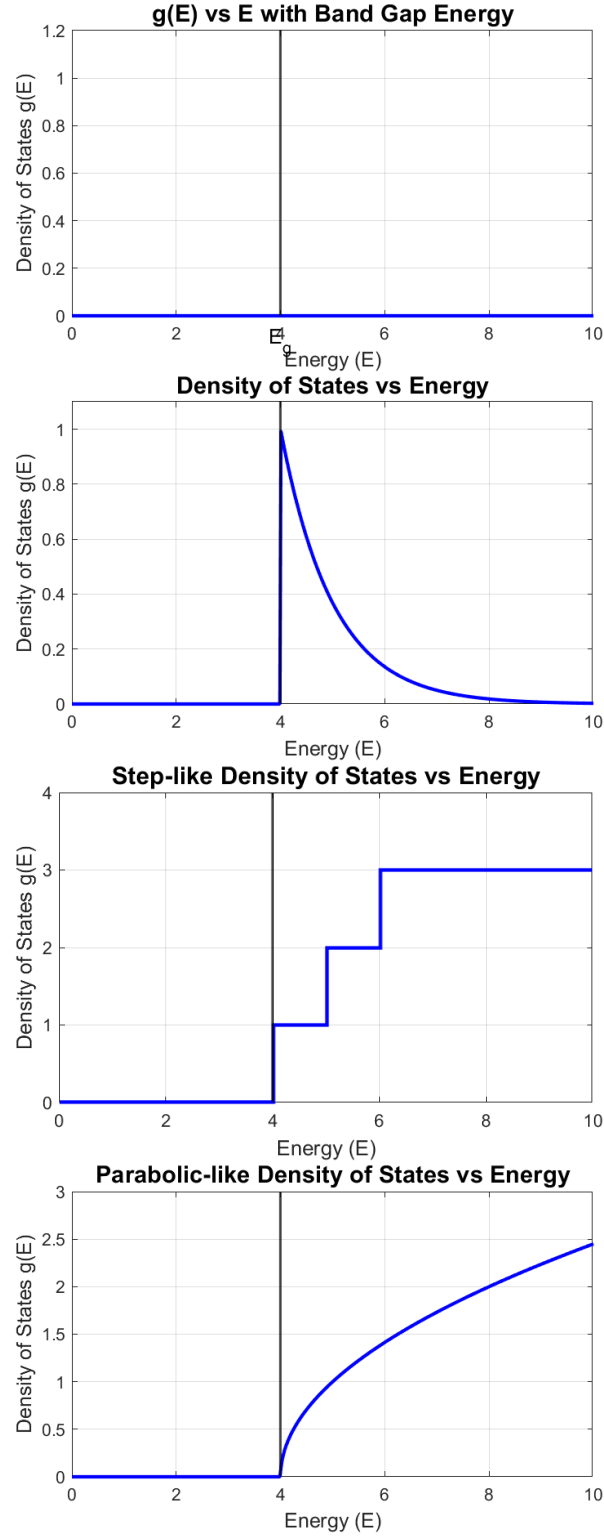


Figure 1: Schematic representation of zero-dimensional (0D), one-dimensional (1D), two-dimensional (2D), and three-dimensional (3D) nanomaterials and density of electron states of a semiconductor by varying dimension, where $g(E)$ is the density of states

On the basis of Confinement	Examples
1D Confinement	Thin film, Quantum Well
2D Confinement	Nanotubes, Nanorods, Quantum wire
3D Confinement	Precipitates, Colloids, Quantum dots

Table 1: An example table.

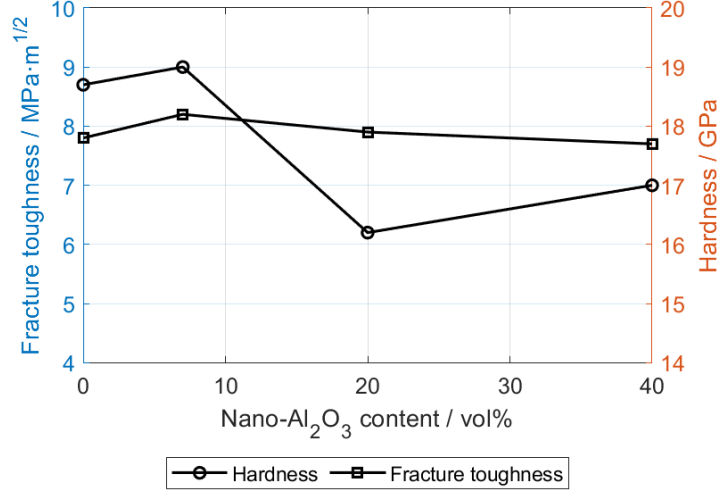


Figure 2: The effects of the content of nano-Al₂O₃ on the fracture toughness and hardness of a ceramic tool material.

2.3 Quantum confinement effects

To confine the movement of random moving electron to restrict its motion in specific energy levels(discreteness). When the particle size is reduced, quantum confinement start becoming dominant, it makes energy levels discrete, energy gap also widen up which leads to discrete electronic energy levels. Nanomaterial is also classified on the basis of Quantum Confinement, look at the Table 1.

2.4 Mechanical Properties

Nanoparticles (NPs) differ from bulk materials, offering a large surface area and enhancing hardness, adhesion, and elasticity. Inorganic NPs improve the weaker mechanical properties of organic compounds. Bui et al. found that adding SnO₂ to acrylic polyurethane boosted hardness, impact, and abrasion resistance, but excessive metal oxides can weaken polymer interactions and cause agglomeration. NP size also affects mechanical properties.

Figure 1 shows the variation law of fracture toughness and hardness with the increase of nano-Al₂O₃ content. The fracture toughness and hardness obviously decrease after initially increasing with the increase in nano-Al₂O₃ content. When the nano-Al₂O₃ content reaches 4 vol.% its fracture toughness and hardness reach the maximum. Therefore, adding a lot of nanoparticles to the matrix may reduce the mechanical properties of a nanocomposite. [3]

3 Chemical Properties

3.1 Chemical Structure and Composition of Nanomaterials

Nanomaterials have complex surface and internal structures, often with multilayers and phases that influence their properties. External factors like temperature and pressure affect atomic arrangements, leading to different crystal structures with varying physiochemical properties (e.g., reactivity, photocatalytic activity). Titania (TiO₂), for example, exists in polymorphs such as rutile, anatase, and

brookite, each with distinct lattice structures and properties. At the nanoscale, anatase shows superior antibacterial and photocatalytic activity due to lower surface energy.

Similarly, carbon exhibits various allotropes (diamond, graphite, CNTs, fullerenes) with unique electrical, mechanical, and chemical properties, based on its covalent bonding. CNTs have diverse forms (armchair, zigzag, chiral) and exceptional strength due to their atomic arrangement. Nanomaterial properties also depend on chemical composition, with crystallites organized into families, such as semicrystalline polymers with distinct crystalline and non-crystalline regions.

3.2 Catalytic Reactivity

Nanomaterials exhibit high catalytic reactivity due to their high surface energy, large surface area, and unsaturated surface atoms, though this also reduces their stability. Their small size maximizes surface atoms—e.g., a 1 nm crystal has 100% surface atoms, compared to 15% in a 10 nm crystal—enhancing chemical interactions.

Nanoparticles act as excellent heterogeneous catalysts, enabling chemical reactions under mild conditions, unlike bulk materials. Their unique electronic structure, driven by quantum confinement and dangling bonds (incomplete surface bonding), increases reactivity. Higher surface energy encourages interaction with external substances, while defects (e.g., vacancies) further enhance reactivity by creating unsaturated atoms with high energy states. These factors make nanomaterials highly effective for catalytic applications.

3.3 Magnetic Properties

As NPs get smaller, they exhibit superparamagnetism, where random magnetic moment flipping occurs, and they show high magnetization only when an external magnetic field is applied. When the field is removed, they retain no magnetization. This contrasts with bulk materials, which may have multi-domain structures.

Magnetic elements like Fe, Co, and Ni are typically used, but at the nanoscale, even diamagnetic elements such as Sc, Zr, and Ti can exhibit magnetism due to uneven electron distribution. The magnetic properties of NPs are influenced by factors like size, shape, composition, and crystallographic structure.

Two important parameters influencing NP magnetism are size and shape. Refer to Figure: 3 Below a critical radius (r_c), NPs form single-domain structures, which increase coercivity as the NP size increases. Above the critical radius, multi-domain structures form, reducing coercivity. Shape also affects coercivity, with cubic NPs showing lower coercivity than spherical ones due to surface pinning effects. The composition and magnetocrystalline phase also play roles, as bimetallic NPs can display superparamagnetic behavior depending on their structure.

3.4 Optical properties

The optical properties such as reflection, transmission, absorption, and light emission of the nanomaterials are completely dependent on their electronic structure that significantly differs for various morphologies since electronic structure of the nanomaterials are very much dependent on surface atoms. Two factors, namely, increased energy level spacing (quantum effect) and surface plasmon resonance, profoundly contribute to the size-dependent optical properties of nanomaterials. Size effects on optical properties are observed when the particle size is reduced to 10nm. This optical bandgap increases with the decrease in particle size, especially for the semiconductor nanomaterials. [1]

One of the most excellent properties of AuNPs is its optical properties. AuNPs are mostly observed in the brown, orange, red, purple and blue color range. Refer to Figure: 4 The color of the molecules is affected by particle aggregation. For examples, AuNPs in the solution has red color, the aggregation leads the absorption intensity increased and changed the colors to blue. The absorption of certain wavelengths in colloidal AuNPs results in vibrant colors due to surface plasmon resonance, known as SPR absorption. The SPR absorption peak of AuNPs is dependent on AuNP particle size. For example, 13nm spherical AuNPs absorb the highest peak at around 520 nm, while 99 nm AuNPs absorb at 600 nm. Kneipp et al. and Nie et al. further apply the unique SPR effect of AuNPs in probes for single molecule surface enhanced Raman scattering or SERS detection. This characteristic makes AuNPs effective tools in protein detection.

The change³ in magnetic coercivity of NPs as a function of particle radius.

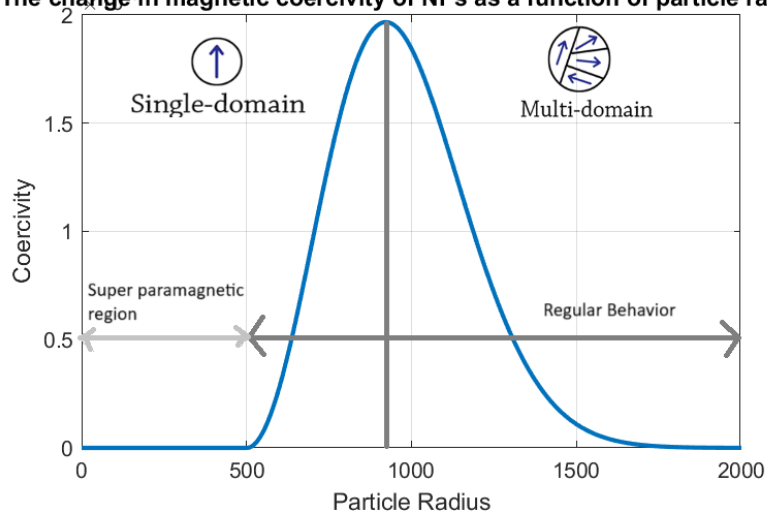


Figure 3: Magnetic Behavior

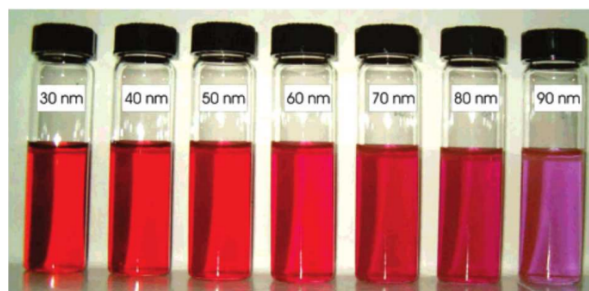
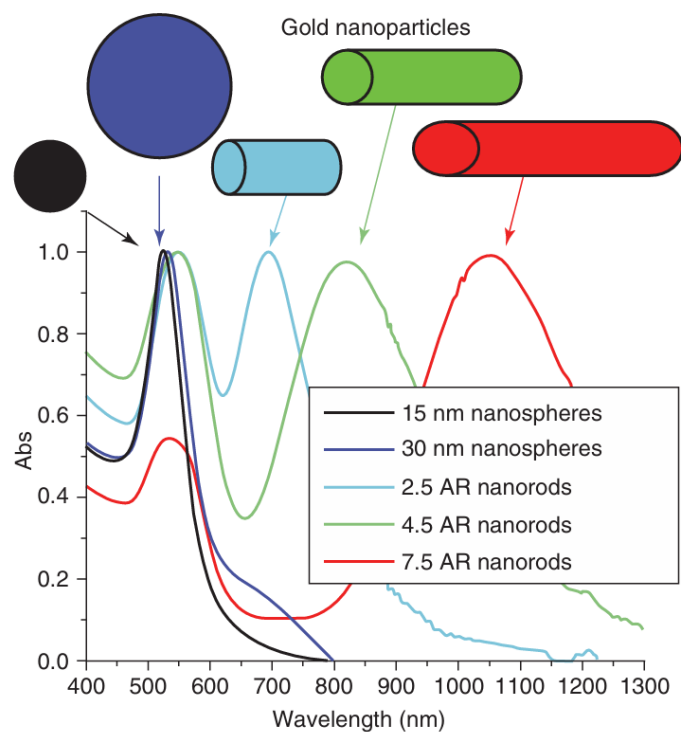


Figure 4: Influence of gold shape on color change. Source: Adapted with permission from Eustis and El-Sayed [24], Copyright © 2005, RSC.

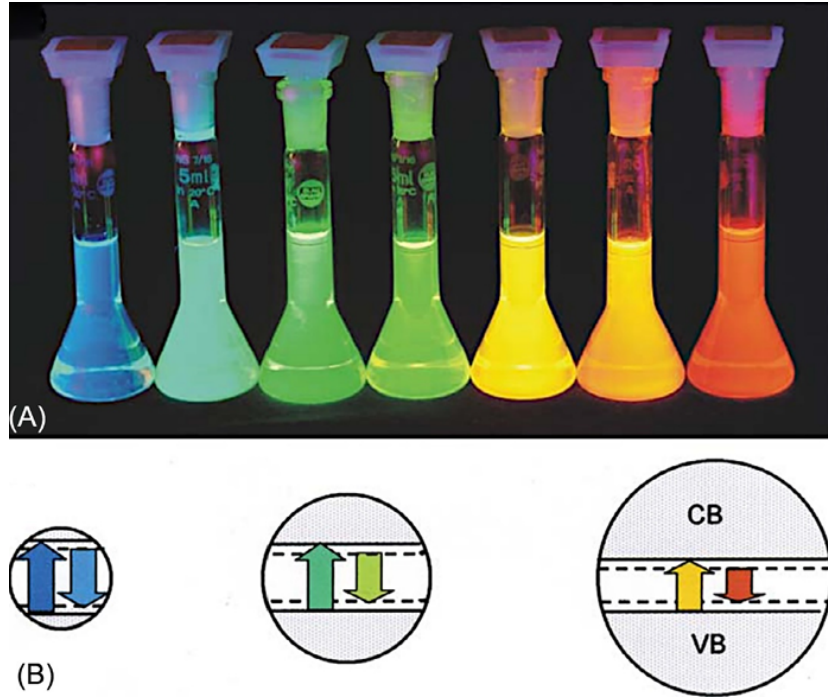


Figure 5: (A) Fluorescence of CdSe-CdS core-shell nanoparticles with a diameter of 1.7nm (blue) up to 6nm (red), giving evidence of the scaling of the semiconductor bandgap with particle size. (B) Schematic representation of the size effect on the gap between the valence band (VB), the conduction band (CB), the absorption (up arrow) and fluorescence (down arrow). Smaller particles have a wider band gap.

Nanosized gold has another very particular behavior. It is well known that gold is considered chemically inactive; however, it was recently reported that gold nanoparticles, i.e. less than 2nm, show an unexpected antimicrobial effect toward Gram-positive and Gram-negative bacteria. This broad antimicrobial activity was attributed to the ability of ultra small gold nanoparticles to interact with bacteria leading to a metabolic imbalance and a high production of reactive oxygen species (ROS) that kills the bacteria. It should be quite evident from the above reported examples that the behavior and the properties of nanomaterials are much more because of the size and surface area rather than to their chemical composition.

3.5 Vibrational and Thermodynamic Properties

A simple theoretical model is developed to study the size and shape dependence of Debye temperature, Debye frequency, melting entropy, and melting enthalpy of nanomaterials. The model is based on the relations between the Debye temperature, Debye frequency, melting entropy, and melting enthalpy of bulk materials and nanomaterials. θ and ν are the Debye temperature & frequency respectively.

$$\frac{\theta_{Dn}}{\theta_{Db}} = \sqrt{1 - \frac{N}{2n}} \quad (1)$$

$$\frac{\nu_{Dn}}{\nu_{Db}} = \sqrt{1 - \frac{N}{2n}} \quad (2)$$

Key findings: ...

1. The Debye temperature, Debye frequency, melting entropy, and melting enthalpy are found to decrease with decreasing size, and the trend of variation is similar in all three shapes (Spherical, Nanowire and Nanofilm).
2. The melting entropy is found to decrease with decreasing the size of the materials.

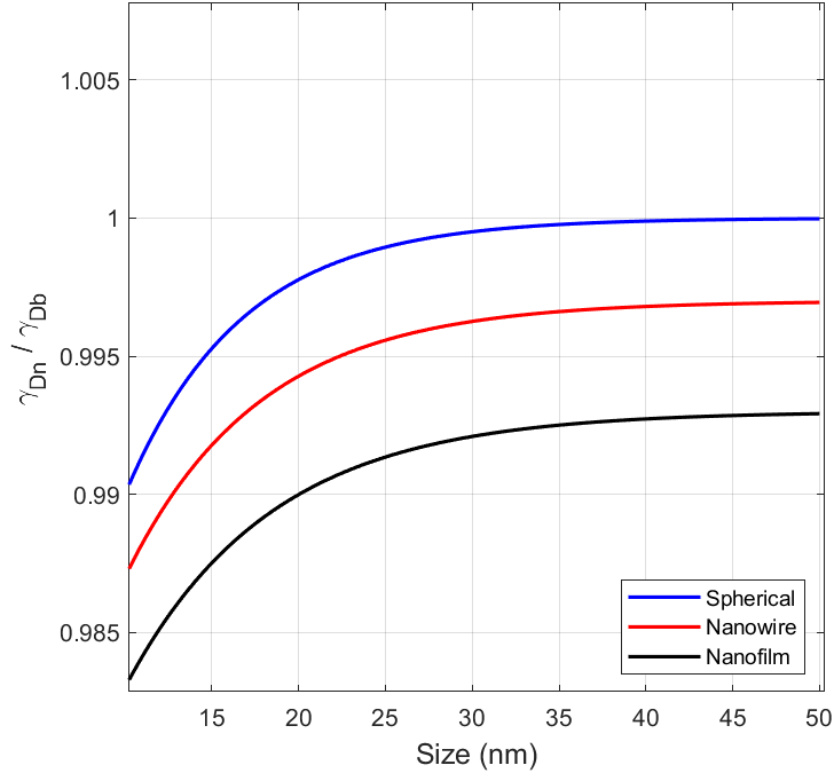


Figure 6: Size and shape dependence of Debye frequency of $\beta - Fe$

3.6 Conclusion

Nanomaterials exhibit a wide range of unique physical, chemical, and mechanical properties that differ significantly from their bulk counterparts due to their nanoscale size. These properties—such as quantum confinement effects, high surface-to-volume ratio, and superparamagnetic behavior—make nanomaterials highly versatile for various applications, including catalysis, electronics, and biomedicine. The ability to manipulate the size, shape, and composition of nanomaterials enables precise control over their optical, magnetic, and catalytic properties, which is essential for innovative advancements in technology and research. Continued exploration into the behavior of nanomaterials, particularly regarding their mechanical strength, reactivity, and thermal stability, holds great promise for the future of material science, contributing to the development of more efficient, durable, and sustainable solutions across numerous industries.

4 Codes of All schematic diagrams

All codes are available on my [GitHub Repository](#), Each file is in the format of MATLAB(.m), you can download zip file, then copy and paste in your MATLAB software.

References

- [1] Anika Benozir Asha and Ravin Narain. Nanomaterials properties. In *Polymer science and nanotechnology*, pages 343–359. Elsevier, 2020.
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- [3] Qiong Wu, Wei-shou Miao, Yi-du Zhang, Han-jun Gao, and David Hui. Mechanical properties of nanomaterials: A review. *Nanotechnology Reviews*, 9(1):259–273, 2020.