PROPERTIES OF NANOMATERIALS

- **Nanomaterials have properties that are different from those of bulk materials.**

- **Most nanostructure materials are crystalline in nature and they have unique properties.**

PROPERTIES OF NANOMATERIALS

- Certain structures exist only in the nanoscale (i.e. there are no bulk counterparts to these structures).
  - Examples◊ carbon nanotubes (CNTs), Fullerenes, carbon onions etc.
- Certain properties arise only in the nanoscale (i.e if the size of the relevant unit is made larger the property under consideration would not be observed).
  - Examples◊ super-hydrophobicity, super- catalytic activity, superparamagnetism, giant magneto resistance etc.
- Certain combination of properties can only be obtained with nanomaterials and nanostructures
  - Example◊ Abalone shell has a fracture toughness reaching more than 1000 times that of calcium carbonate the chief ingredient in the shell; while still retaining the hardness of nacre.
- Drastic change in properties may be observed on approaching the nanoscale
  - Example◊ Fracture strength of Ni has shown to increase from 100 MPa to 900 MPa once the nanometer-sized grains are obtained.
- The performance of some systems depend on a functional entity in the nanoscale
  - Example ◊ A devise sensing a signal from a single DNA strand has to be in the nanoscale so as to extract the local signal from one strand. Nanoscale entity (such as CNTs) can be utilized for measuring the electrical signal in response to a stimulus.
- In multi-lengthscale structures (with special properties) the fundamental unit has to be nanoscale for the other lengthscales to be effective
  - Example ◊ non-buckling nano-hairs are at the heart of the hierarchical structure on a lotus leaf, which gives it superhydrophobicity.

PHYSICAL PROPERTIES

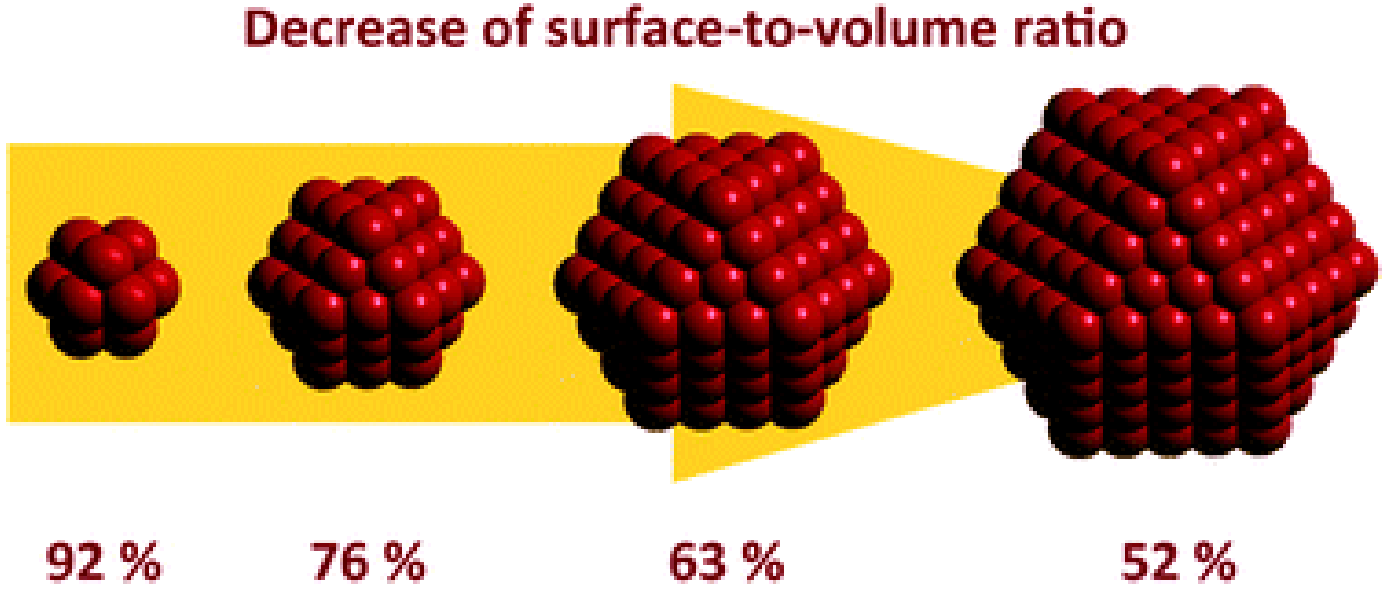
- **Crystal structure of nanoparticles is same as bulk structure with different lattice parameters.**

- **The inter-atomic spacing decreases with size and this is due to long range electrostatic forces and the short range core-core repulsion.**

- **The melting point of nanoparticles decreases with size.**

CHEMICAL PROPERTIES

- A **large fraction of the atoms** are located at the **surface of the nanomaterial** which increase its **reactivity** and **catalytic activity**.
- The large surface area to volume ratio, the variations in **geometry** and the **electronic structure of nano particles** have a strong effect on catalytic properties.



ELECTRICAL PROPERTIES

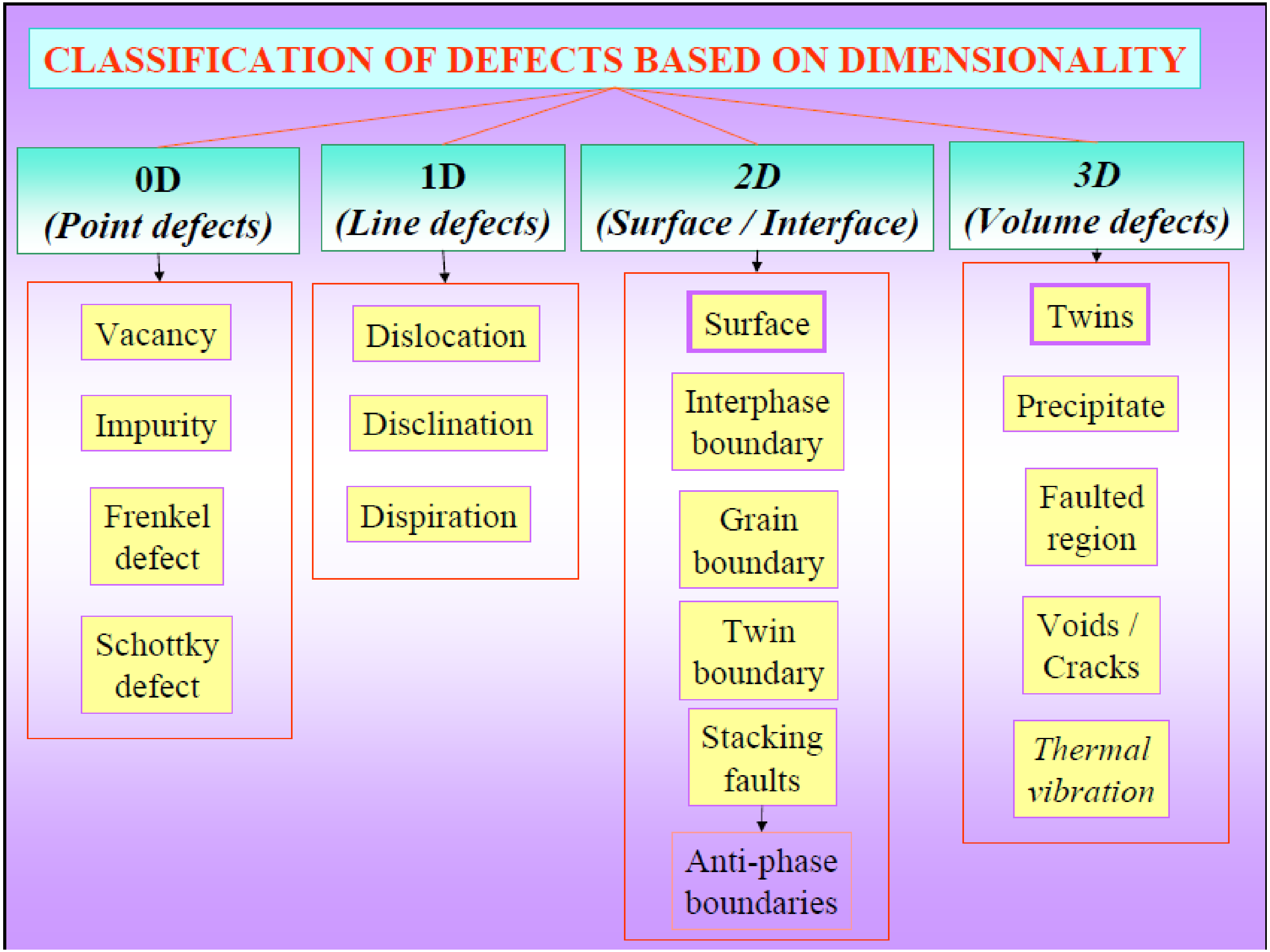
- **The energy band structure and charge carrier density in the materials can be modified quite differently from their bulk and in turn will modify the electronic properties of the materials.**

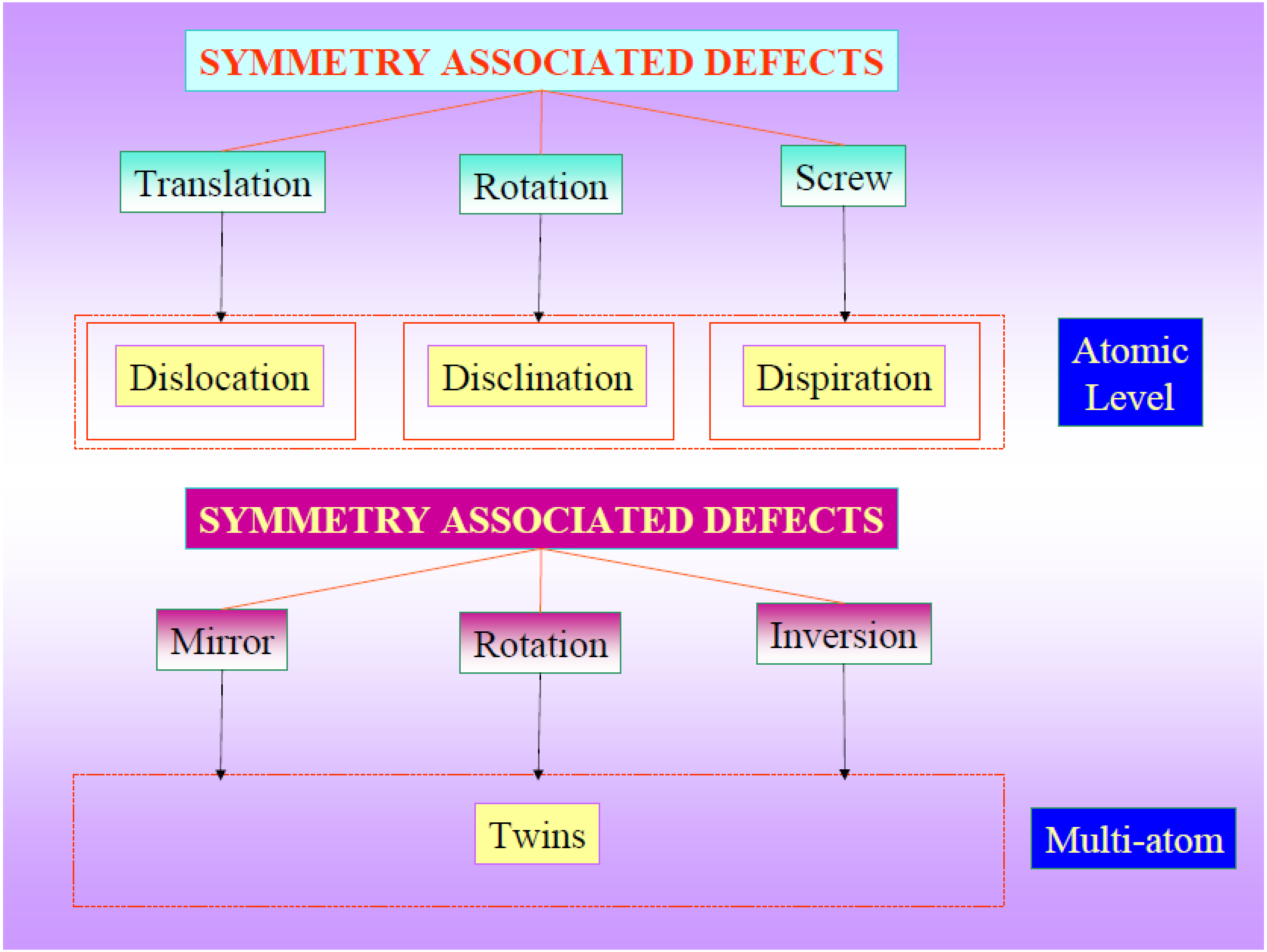
- **Nanoparticles made of semiconducting materials like Germanium, Silicon and Cadmium are not semiconductor.**

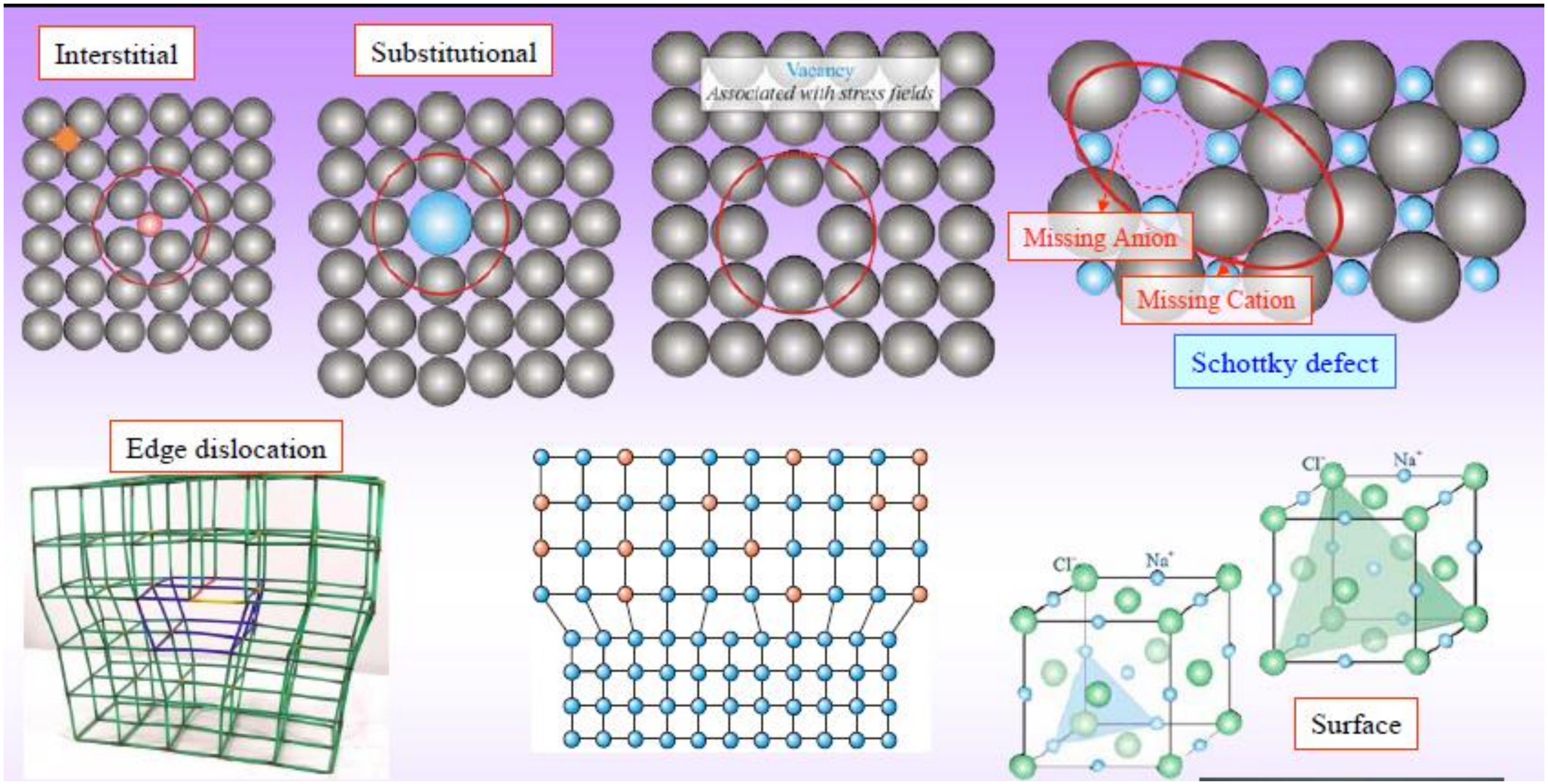
- **Nanoclusters of different sizes will have different electronic structures and different energy level separations. So they show diverse electronic properties which depend on its size.**

- In bulk materials conduction electrons are delocalized and travel ‘freely’ till they are scattered by phonons, impurities, grain boundaries etc.
- In nanoscale conductors two effects become important:
  - Quantum effect: Continuous (‘nearly’) bands are replaced with discrete energy states
  - Classical effect: mean free path (MFP) for inelastic scattering becomes comparable to the size of the system (can lead to reduction in scattering events).
- In metals: change in DOS on reduction of size of the system plays a major role (along with change in electronic and vibrational energy levels).
- In semiconductors quantum confinement of both the electron and hole leads to an increase in the effective band gap of the material with decreasing crystallite size.
- These effects can lead to altered conductivity in nanomaterials.

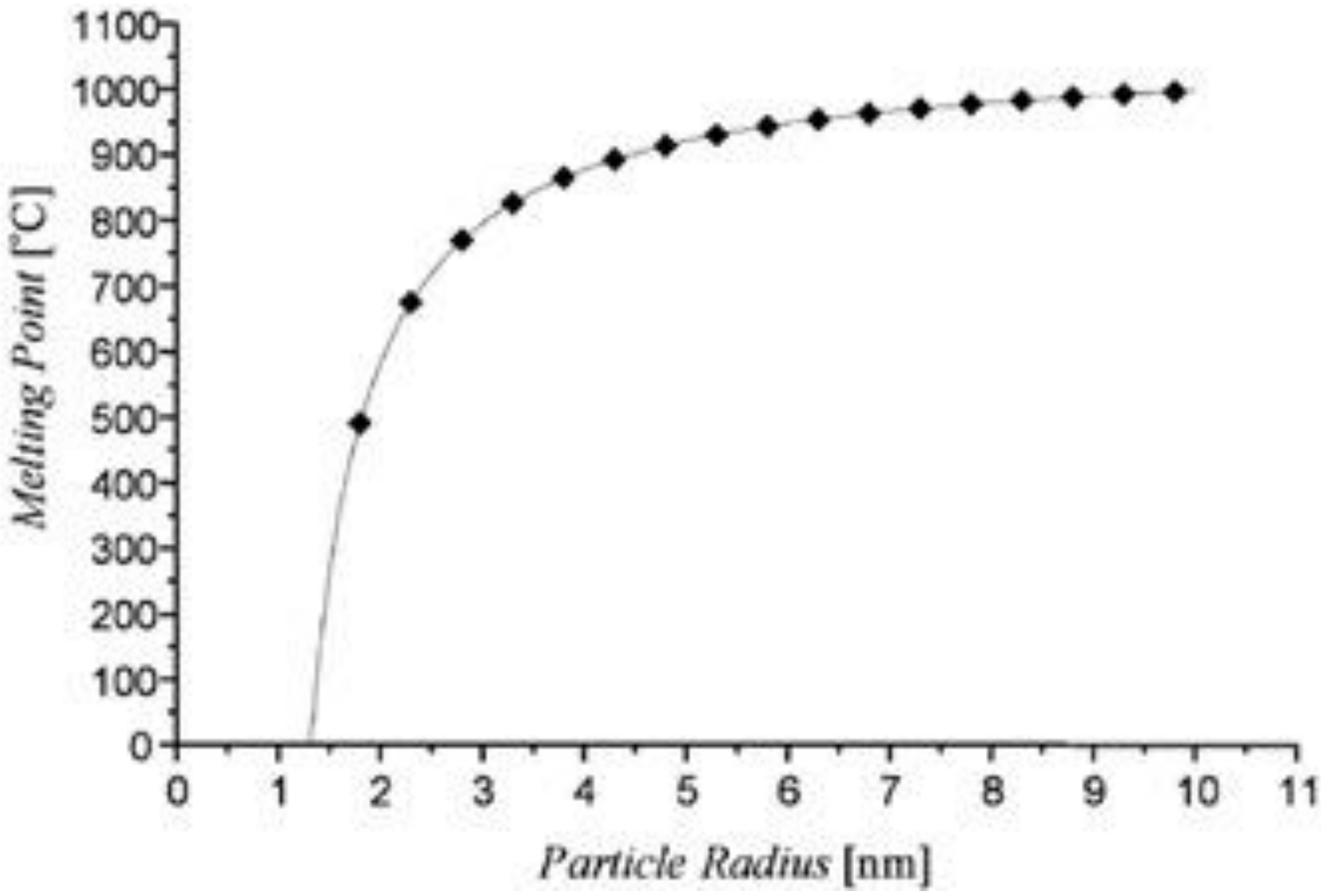
MECHANICAL PROPERTIES




SYMMETRY ASSOCIATED DEFECTS
Translation
Rotation
Screw
Dislocation
Disclination
Dispiration
Atomic Level
SYMMETRY ASSOCIATED DEFECTS
Mirror
Rotation
Inversion
Twins
Multi-atom


Interstitial
Substitutional
Vacancy
Associated with stress fields
Missing Anion
Missing Cation
Schottky defect
Edge dislocation
Cl-
Na+
Cl-
Na+
Surface

- Melting point of a material is an indicator of the bond strength of a material (though boiling point is better reference as it is structure independent).
- In bulk systems surface to volume ratio is small and curvature effects can be ignored.
- In nanocrystals the number of surface atoms is a considerable fraction of the total number of atoms. These atoms have a higher energy and higher freedom for vibrations.
  - This implies that surface atoms *are expected* to melt below the melting point of the bulk.



MAGNETIC PROPERTIES

- **The magnetic moment of nano particles is found to be very less when compared them with its bulk size.**

- **It should be possible that non-ferromagnetic bulk exhibit ferromagnetic-like behavior when prepared in nano range.**

- **Bulk Gold and Pt are non-magnetic, but at the nano size they are magnetic.**

Even in bulk magnetic materials some structures can be in the nanoscale:

- Domain walls in a ferromagnet (~60nm for Fe).
- Some domains (especially those in the vicinity of the surface or grain boundaries), could themselves be nanosized.
- Spin clusters above paramagnetic Curie temperature (θ_p) could be nano-sized.

When we go from bulk to 'nano' only the structure sensitive magnetic properties (like coercivity) is expected to change significantly.

Some of the possibilities when we go from bulk to nano are:

- Ferromagnetic particles becoming single domain
- Superparamagnetism in small ferromagnetic particles (i.e. particles which are ferromagnetic in bulk)