Why are the properties of nanophase materials unpredictable?

The uncertainty in logically predicting the properties of nanophase materials arises from the sudden changes in structure–property relationships at nano-scale.

Properties of matter in bulk scale broadly fall into two categories:

- Intrinsic properties: These are the properties essential to the nature, character or identity of the material. These properties are (largely) independent of size or shape of the material. E.g. Glass transition temperature of a polymer, surface tension, hardness, conductivity, magnetism, color, refractive index, melting point and chemical activity. Materials derive these properties from the basic chemical factors such as electronic configuration, nature of chemical bonding, molecular weight or lattice structure. Intrinsic properties thus may be looked upon as signature of the material.
- Extrinsic properties: These are the properties in bulk state which for a given material do vary with the particle size, its distribution, surface area and shape in accordance with the well understood relationships. E.g. Tinting strength, opacity, oil absorption of pigments, adsorption capacity, and catalytic capacity.

In the domain of nanosize, as we know, the surface area to volume ratio shows sharp increase and surface atoms dominate the properties of the material due to their higher population. There is an increase in energy inversely proportional to the square of length scale. This energy is dissipated by building new structures within the nanophase as well as with the surrounding matrix. This phenomenon leads to drastic change in the properties of the material. Intrinsic properties turn into extrinsic size-dependent characteristics, e.g. higher surface tension and lower melting points at nanoscale. Extrinsic properties also change as an exponential function of surface area, e.g. adsorption capacity is much greater in nanostructures. Thus, the properties exhibited by the nanophase are a combined effect of some intrinsic properties becoming extrinsic and the extrinsic properties getting greatly enhanced. Since the frame work of rules governing these complex changes is not yet fully established, prediction of properties is very difficult.

To understand the complexity, let us look at the following empirical observations:

- Even within the nano-scale region, the properties of materials do vary significantly with the particles size.
- Two properties which are related in a known way in the bulk scale can show opposite behavior in the nanoscale, e.g. While thermal and electrical conductivity go in tandem in the bulk state, it is possible to design nanomaterials with poor thermal conductivity and excellent electrical conductivity.

Great deal of fundamental research is presently devoted to establishing structure property- relationships of different materials in the nano region. The scientists have spoken about different 'Periodic Tables' depending on particle size in nano range for the existing elements. It is estimated that it may take until the year 2015 for more complete theoretical understanding of nano-size phenomena to emerge.

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