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DISCUSSION ABOUT THE PROPERTIES OF NANO-CRYSTALS AND CONCEPT OF BULK SOLIDS APPLICATION & PROPERTIES

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ABSTRACT

Nanoparticles' small size, high surface area, and composition all contribute to their distinctive thermodynamic characteristics. For many applications in nanoscience and nanotechnology, it is crucial to comprehend and correctly predict these features. In this abstract, a model for examining the thermodynamic characteristics of nanoparticles while taking into account their size, shape, composition, and surface effects is presented. The model makes use of theoretical frameworks from quantum mechanics and statistical mechanics to account for the impacts of size-dependent phenomena, such as quantum confinement and surface energy. It takes into consideration various materials, alloys, or core-shell architectures to account for the composition of nanoparticles. The model incorporates the qualities that depend on composition, such as binding energy and interatomic interactions.

Keywords: - Nanoparticles, Thermodynamic, Nanoscience, Nanotechnology, Properties

I. INTRODUCTION

The idea of nanotechnology first appeared in the famous talk "there is plenty of room at the bottom" given by the physicist Richard Feynman at the American Physical Society meeting at Caltech on December 29, 1959. Feynman anticipated and described a process by which scientists would acquire the ability to manipulate materials at a nanoscale, and indeed he was right because here we are the 21st century doing just that. The term nanotechnology was originally defined by Norio Taniguchi in 1974 as follows: "nanotechnology mainly consists of the processing of separation, consolidation and deformation of materials by one atom or by one molecule." Nanotechnology and nano science began in the early 1980's with the advances in computing power and material modelling. Nano-materials are basically the link between nano science and nanotechnology. Nano-materials generally deal with sizes less than 100nm.

With the development of nano science and nanotechnology in recent years, size of materials come into nano meter size range (<100nm) at least in one dimension. This leads to dramatic increase of surface/volume ratio and corresponding changes of physical, chemical and mechanical properties. It is very important to understand these properties and their related physical basis for correct industrial application.

II. THERMO PHYSICAL PROPERTIES OF NANO-CRYSTALS

The theoretical and experimental studies on electrical, mechanical, optical and thermal properties of nano-materials have been of great interest world-wide during the last decade. The physical and chemical properties of nanomaterials have been widely investigated because of their industrial and scientific applications. The nanomaterials differ from the corresponding bulk form of material mainly due to their small size. The physical parameters like melting temperature, cohesive energy, activation energy, energy band gap and Young's modulus remains constant for bulk material at normal conditions, however, these parameters are found to change with the reduction in size of material to nano level.

Cohesive energy of material varies with grain size and hence melting temperature gets affected. Melting-point gets reduced as particle size is reduced and thus the thermal properties of nano materials show different behaviour as compared to its bulk form. This is probably due to increase in the ratio of surface area to volume in nano materials. The surface area of differently shaped nano crystals is different and hence the physical properties of the nano crystal vary with shape and size. It is, therefore, pertinent to consider both shape and size effect for understanding the properties of materials at the nano level. In order to understand the impact of shape and size on nano materials, the expression of cohesive energy is shown in terms of number of surface atoms and interior atoms in the nanomaterial. In past years, several theoretical simulations and experimental work have been carried out to study the thermo-physical properties of nano materials. The bottoms up as well as top down approaches are applied to study the change in thermodynamic properties of solid nano materials. Top down approaches are mostly based on classical thermodynamics and bottom up approaches are based on complicated simulations.

III. EFFECT OF SHAPE AND SIZE

The bulk properties of crystals depend on their structure, but at the nanoscale, in addition to the structure, their size and shape are an important factor, which influences their properties. The most significant characteristic of materials at the nanoscale is their high surface to volume ratio, which affects their thermodynamical properties. It is now well known that the melting temperature of nanoparticles depends on their size. Melting temperature depression occurs for almost all free nanoparticles and superheating has been reported for nanoparticles embedded in other host materials.

There are relatively extensive investigations on the size dependence of melting and cohesive energy of nanocrystals. However, it has not been accompanied by the necessary investigation of size dependence of vibrational properties and thermodynamics of nanocrystals. Such investigations should depend on our understanding of the size effect of melting and cohesive properties. In particular, a

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complete understanding of the melting transition in nanocrystals cannot be obtained without a clear understanding of enthalpy and entropy of melting, which are important properties of melting,

The effects of particle size and thermodynamic energy, based on surface thermodynamics and the atomic bond energy, were used to calculate the mechanical properties, such as surface tension and Young's modulus of nanocrystals. The cohesive energy is the basic thermodynamic property used to predict melting temperature, melting enthalpy, melting entropy and specific heat of nanomaterials. Scholars have proposed different models, namely the latent heat model, the liquid drop model and the surface area difference model, to predict cohesive energy of nanomaterials. Recently, using the concept of cohesive energy changes with the atomic coordination environment, Qi presented a theory based on the bond energy model to highlights the thermodynamics for the nanoparticles, nanowires, and nanofilms. The size and coherence dependent cohesive energy, melting temperature, melting enthalpy, vacancy formation energy and vacancy concentration of nanowires and nanofilms have been reported. The variation direction of the thermodynamic properties is observed to be determined by the coherent interface and the quantity of variation depends upon the crystal size. Shandiz et al. developed a model for melting entropy and enthalpy of metallic nanoparticles, which is based on the effect of packing factors, coordination numbers of lattice and crystalline planes. Thus, it appears that there exist some attempts to study size-dependent thermodynamical properties. Moreover, because the thermodynamical properties also depend on the shape, it may be valuable to present a model that incorporates the effects of shape.

IV. CONCEPT OF BULK SOLIDS

Bulk solids, also known as granular materials or powders, are a class of materials consisting of a collection of solid particles. They are characterized by their ability to flow under the influence of gravity and their interactions with each other. Bulk solids can range from fine particles like flour or cement to larger particles like gravel or coal. They play a crucial role in various industries, including agriculture, pharmaceuticals, mining, food processing, and construction.

Properties of Bulk Solids:

- Particle Size and Size Distribution: Bulk solids can have a wide range of particle sizes, from nanoparticles to larger particles. The size distribution of particles within a bulk solid affects its flow ability, packing density, and other properties.
- Particle Shape: Particle shape influences the flow behaviour and interlocking between particles. Irregularly shaped particles may exhibit greater interlocking, leading to increased cohesion and reduced flow ability.
- Particle Density: Bulk solids have a bulk density, which is the mass of the solid particles divided by the total volume, including the void spaces between particles. Particle

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density affects the flow properties and compressibility of bulk solids.

Challenges in Handling Bulk Solids:

Handling and processing bulk solids present several challenges due to their complex behaviour. Some common challenges include:

- Flowability Issues: Bulk solids may experience flow problems such as bridging, rat-holing, or arching, which can disrupt material flow and cause blockages in storage or conveying systems.
- Segregation: Segregation can occur during storage or handling, leading to uneven distribution of particle sizes or components. This can impact product quality, performance, or downstream processes.
- Dust Generation: Many bulk solids can generate dust during handling, which poses health and safety hazards, as well as potential explosion risks.

Applications

Bulk solids find a wide range of applications across various industries. Some common applications of bulk solids include:

- Food and Beverage Industry: Bulk solids such as grains, flour, sugar, spices, and powdered ingredients are widely used in food processing, baking, confectionery, and beverage production.
- Pharmaceutical Industry: Bulk solids like powders, granules, and tablets are used in the manufacturing of pharmaceutical drugs, including tablets, capsules, and oral powders.
- Chemical Industry: Bulk solids are used as raw materials, catalysts, fillers, or additives in the chemical industry. Examples include powders for paint and coating formulations, plastic pellets, and catalyst particles.

V. NANO MATERIALS

Nano materials, also known as nanomaterials, are materials with structures and properties at the nanoscale level. The term "nanoscale" refers to dimensions typically between 1 and 100 nanometers (nm), where 1 nanometer is equal to one billionth of a meter. At this scale, materials exhibit unique physical, chemical, and biological properties that differ from their bulk counterparts. Nano materials have gained significant attention and hold great potential for various applications in fields such as electronics, energy, medicine, and environmental remediation.

Properties

Nano materials exhibit unique properties at the nanoscale due to their small size, high surface-to-volume ratio, and quantum effects. The properties of nano materials can vary depending on their composition, structure, and fabrication methods. Here are some key properties of nano materials:

- **Size-Dependent Properties**

The properties of nano materials are strongly influenced by their size. As the size decreases to the nanoscale, the materials may exhibit different electronic, optical, magnetic, and mechanical behaviors compared to their bulk counterparts.

- **Enhanced Surface Area**

Nano materials have a significantly increased surface area compared to their volume. This high surface-to-volume ratio leads to enhanced reactivity, adsorption capacity, and interaction with surrounding environments.

- **Quantum Effects**

At the nanoscale, quantum effects become prominent, and the behavior of nano materials is governed by quantum mechanics. Quantum confinement and quantum size effects can result in unique optical, electronic, and catalytic properties.

- **Mechanical Properties**

Nano materials can exhibit improved mechanical properties, such as increased strength, hardness, and flexibility. The presence of nanoscale grain boundaries and defects can affect the deformation mechanisms and mechanical behavior.

Electrical and Electronic Properties: Nano materials can display altered electrical conductivity, resistivity, and bandgap properties. Quantum confinement can lead to changes in electronic band structures, allowing for the tuning of electrical and optical properties.

VI. CONCLUSION

High-pressure research on nanomaterials is an exciting and expansive field of study with several practical and technological implications. Using the Goyal and Guptas EOS (eq. 3.1.5), the first pressure derivative of the bulk modulus may be determined in the current study. The modified variants of this equation of state are helpful for investigating the behavior of nanomaterials under high pressure compression. Because it is founded on the rules of thermodynamics, the equation of state may be used to extrapolate to regions for which experimental evidence is lacking.

For the investigation of thermodynamically and optical characteristics of nanomaterials, such as melting enthalpy, Debye temperature, specific heat, bandgap expansion, vibrational frequency, electrical susceptibility, and dielectric constant, the Guisbiers model (eq. 3.2.4) is determined to be the optimal equation. The melting point and cohesive energy of nanomaterials may also be investigated using the liquid drop model. It is also possible to determine the Curie temperature of nanomaterials by employing the Bond energy model. In this work, it is reported that the computed values correspond well with the experimental ones. Simple methods for calculating nanomaterials' thermophysical characteristics have been published.

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