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A QUANTUM THERMODYNAMIC MODEL FOR THE MELTING TEMPERATURE OF CYLINDRICAL AG NANOPARTICLES DEPENDENT ON THEIR SIZE AND SHAPE

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ABSTRACT

In this study, we propose a numerical thermodynamic model to investigate the melting temperature dependence on particle size and shape for nanoparticles. The model specifically considers silver (Ag) nanoparticles in a cylindrical form. By integrating size and shape parameters, we provide a comprehensive analysis of the melting behavior, which is crucial for applications in nanotechnology where thermal stability is a key factor. The results demonstrate significant variations in melting temperatures with changes in nanoparticle dimensions, offering valuable insights for the design and utilization of nanomaterials in various technological applications.

Keywords: Nanoparticles, Temperature, Particle, Shape, Thermodynamic.

I. INTRODUCTION

Nanoparticles exhibit unique physical and chemical properties that differ markedly from their bulk counterparts, making them valuable in a wide range of technological applications, from electronics and catalysis to medicine and materials science. Among these properties, the melting temperature of nanoparticles is of particular interest due to its significant implications for their thermal stability and performance in various applications.

The melting temperature of nanoparticles is known to depend on several factors, including particle size and shape. Traditional models primarily focus on spherical nanoparticles, providing a limited understanding of how other shapes, such as cylindrical nanoparticles, behave under thermal conditions. This gap in knowledge necessitates the development of more comprehensive models that can accurately predict the melting temperatures of nanoparticles with diverse geometries.

Silver (Ag) nanoparticles are especially noteworthy due to their exceptional electrical conductivity, antimicrobial properties, and catalytic efficiency. Cylindrical Ag nanoparticles, such as nanowires and nanorods, are integral to many cutting-edge applications in nanoelectronics, photonics, and biosensors. Understanding the melting behavior of these cylindrical nanoparticles is crucial for optimizing their thermal stability and performance.

This study aims to address the current knowledge gap by proposing a numerical thermodynamic model that accounts for the particle size and shape dependent melting temperature of cylindrical Ag nanoparticles. Our

model integrates thermodynamic principles with numerical techniques to analyze how variations in size and shape influence the melting temperature of these nanoparticles. By focusing on cylindrical shapes, this research provides new insights into the thermal properties of non-spherical nanoparticles.

The development of this model involves a detailed examination of the interplay between particle size, shape, and melting behavior. The results from this study will enhance the understanding of how cylindrical Ag nanoparticles behave under different thermal conditions, guiding the design and optimization of nanomaterials for various high-performance applications.

II. REVIEW OF RELATED STUDIES

Varotsos, P. et al., (2022) For decades, the question of whether the thermodynamic properties of solid point defects are directly related to the material's bulk properties has been of utmost concern. Researchers over fifty years ago proposed a relationship between the bulk properties of solids and their defect Gibbs energy gi, answering this urgent question. This relationship shows that the gi is directly proportional to the isothermal bulk modulus B and the mean volume per atom, as described by the cB model, for a number of processes (such as defect formation, self-diffusion activation, and heterodiffusion).

According to Ram et al. (2021), An approach to determine the surface contribution to solid thermodynamic properties using a localized frequency spectrum representation is detailed here. An extensive discussion of surface atomic vibrations is provided in the context of the Green function theory of isolated point defects. You may represent the atomic spectra at every point in space as a function of the Green functions at that point. The surface's role in solid thermodynamic properties is shown using local atomic frequency spectra from a few surface layers and the infinite crystal's frequency spectrum that satisfies the cyclic boundary requirement.

Ratan Jaiswal and Brijesh Pandey (2021) Explaining and describing nanoscale thermophysical characteristics is still a difficult problem. Despite the hard work of pioneering workers and scientists, a perfect model for predicting and explaining these traits has yet to be developed. To account for the form effect and the nanoscale structure of materials, a novel model has been suggested in this study for calculating thermophysical parameters such as specific heat, melting enthalpy, and melting entropy. The nature of fluctuation of the aforementioned critical thermodynamic parameters at the nano level has also been predicted using this exciting hypothesis.

Goyal, Monika & Gupta, B. (2020) To investigate how nanowire thermodynamic characteristics change with changes in form, size, and structure, a basic model based on thermodynamic variables is utilised. Cohesive energy is quantified using the formula developed by Qi and Wang, and the ratio of surface atoms to total atoms is written in terms of the shape parameter, the radius of the nanowire, and the atomic packing fraction.

Fu, Qingshan, et al (2018) When it comes to physicochemical changes, the surface thermodynamic properties of nanocrystals are key. It is currently not known how precise regularities in size and form affect the thermodynamic properties of surfaces made of nanocrystals. Hence, by combining the Young-Laplace equation and including interface variables into the Gibbs energy, relationships between the size and surface thermodynamic properties (surface enthalpy, surface energy, surface heat capacity, and surface energy) were determined for nanocrystals of different shapes. There is agreement between theoretical estimations and experimental evidence about the thermodynamic properties of nanocrystal surfaces. Results show that for r >

10 nm, surface thermodynamic properties of Au, Bi, and Al nanocrystals change linearly with the reciprocal of particle size. However, for r 10 nm, the impact of particle size grows and the surface thermodynamic properties show a stronger departure from linear variation. For identically sized non-spherical nanocrystals, the surface thermodynamic properties (absolute value) are larger.

Fu, Qingshan et al., (2017) Nanocrystals (NCs) undergo physicochemical changes that are heavily influenced by their thermodynamic characteristics, particularly their surface thermodynamic properties. However, how size and form regularities affect the thermodynamic characteristics of NCs is yet unknown.

Mengfan Liang, et al (2020) In this research, we used molecular dynamics simulation to examine how different SiO2 particle sizes and shapes affect the interface structure and thermodynamic performance of polyimide (PI)/SiO2 composites. Experiments were also conducted to see if the addition of a nanofiller might significantly improve the interaction between PI and SiO2. The surface of the silica nanoparticle was modified using the coupling agent ICTOS to improve the interfacial intensity efficiency. The results shown that the glass transition temperature of the composites is affected by the size and shape of the SiO2, which in turn affects the interfacial number of hydrogen bonds and the interfacial area. Bonded energy and Tg were shown to decrease with increasing nanosilica radius, indicating a significant filler size impact. While the Tg of spherical-type systems was higher than that of other nanosystems, the reverse was not true.

Ashwini D. Dixit & Rekha S. Sharma (2018) Crystals' structure determines their bulk characteristics, but at the nano scale, their size and shape also play a significant role in determining their properties. A high surface-to-volume ratio, which is a hallmark of nano materials, significantly modifies their thermodynamic characteristics. In order to calculate the melting enthalpy and entropy of nanocrystals, a straightforward model may be constructed using Mott's equation for the melting entropy and the size dependence of the melting temperature. Melting enthalpy in Sn, Ag, and nano-materials of varying forms has been investigated, as have their size and shape dependencies. As particle size is reduced, the melting entropy is observed to decrease. For a certain size, the entropy of a system grows from spherical to nanowire to nanofilm. Reducing a thing's size is also discovered to have a negative effect on its enthalpy.

III. PROPOSED APPROACH

The cohesive energy, also known as bonding energy, is defined here as the product of the total energy released during the formation of a stable bond between the atomic distances and the bond length. To forecast the shape-dependent size influence on nanoparticle temperature, all that is needed is the radius of curvature expression of a cylindrical nanoparticle using the helix approach. In addition, this approach might be tested experimentally by comparing the particle shape with radius of curvature; this would be the focus of future investigations. It is a new parameter for nanoparticle characterization. The nanoparticles' shapes determine their radius of curvature. The size of the particles is determined by the radius of curvature in relation to the inferred melting point.

This study shown that when nanoparticle size was lowered, the melting point dropped. Also, since cylindrical nanoparticles have a higher surface area, this decrease is more pronounced in them than in spherical ones. On a material's surface, an increase reduces the bonding or cohesive energy. For the simple reason that more atoms are exposed to the environment and may form bonds with atoms in the layer below them on a bigger surface. A result is that the surface atoms' cohesive energy is lower than that of the atoms located in the solid's

internal bulk. In order for the surface's atoms to either melt or be displaced. Therefore, the melting point of a solid is lower. A similar phenomenon, strongly correlated with size, was investigated on silver nanomaterial. Since silver has the greatest thermal and electrical conductivity of all metals, we focused our computer investigation on it. Because of this, solder, electrical connections, and PCBs are common uses for silver in electronics.

IV. RESULTS AND DISCUSSION

Table 1 shows the results of the equation with regard to surface area, which yields the cohesive energy per mole of the nanoparticle. The relationship between surface area and cohesive energy of Ag nano-material is shown in Figure 1, which shows that the former decreases as the latter grows. Surface areas ranging from 23.2 nm2/g have a cohesive energy of 810 KJ/mol, while those ranging from 119.6 nm2/g have a cohesive energy of 251 KJ/mol. Cohesive energy increases when nanoparticle surface areas decrease, as seen in the graph and the calculations.

Table 1.1:

Ag nanomaterial cohesive energy vs surface area

S. No.	Surface area (nm /g)	Cohesive energy (KJ/mol)
1	23.2	810
2	49.1	632
3	61.2	562
4	82.9	469
5	95.5	368
6	119.6	251

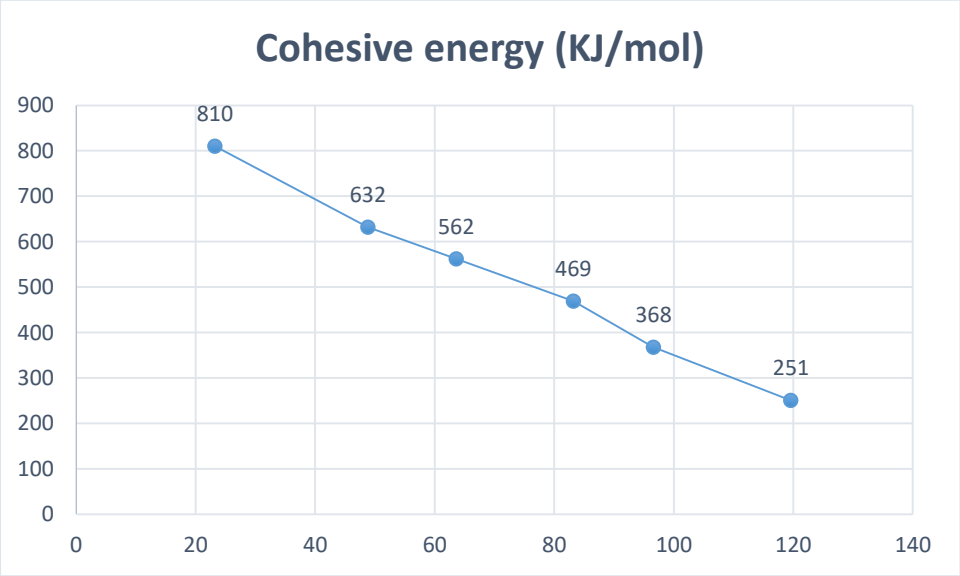

Figure 1.1:

Ag nanomaterial cohesive energy vs surface area

Using the data from the table, the following figure and table show the cohesive energy as a function of particle radius. It has the potential to determine the nanoparticle's size. As the size of the silver nanoparticle shrank from 10.12 nm to 1.57 nm, the surface area grew, and as shown in our study, the cohesive energy dropped from 661 kJ/mol to 292 kJ/mol.

Table 1.2:

Relationship between Cohesive Energy and Particle Radius

S. No.	Cohesive energy (KJ/mol)	Particle Radius (nm)
1	292	1.61
2	330	2.29
3	382	3.36
4	433	4.49
5	468	5.38
6	508	6.20
7	539	6.89
8	588	7.78
9	624	9.02
10	661	10.12

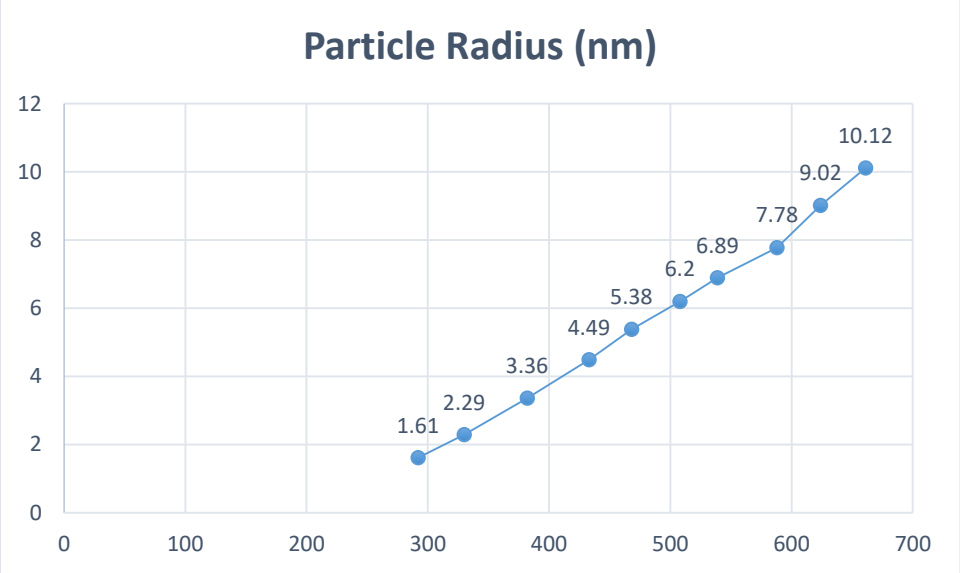

Figure 1.2:

Relationship between Cohesive Energy and Particle Radius

V. CONCLUSION

This study presents a comprehensive numerical thermodynamic model that elucidates the effects of particle size and shape on the melting temperature of cylindrical silver (Ag) nanoparticles. By integrating thermodynamic principles with numerical methods, we have demonstrated that the melting temperature of Ag

nanoparticles is significantly influenced by their size and shape, with cylindrical nanoparticles exhibiting distinct melting behaviors compared to their spherical counterparts.

Our model reveals that as the size of cylindrical Ag nanoparticles decreases, their melting temperature also decreases, highlighting the size-dependent nature of this property. Additionally, the cylindrical shape introduces unique thermal characteristics that differ from those of spherical nanoparticles, emphasizing the need for shape-specific models in nanoparticle research.

The findings from this study provide valuable insights into the thermal stability of cylindrical Ag nanoparticles, which are critical for their application in nanoelectronics, photonics, and other advanced technologies. Understanding the melting behavior of these nanoparticles aids in optimizing their design and enhancing their performance under varying thermal conditions. Future research can build upon this model to explore other shapes and materials, further expanding our understanding of nanoparticle melting behavior. This study underscores the importance of considering both size and shape in the development of predictive models for nanoparticle properties, paving the way for more accurate and application-specific nanomaterial design.

In conclusion, our numerical thermodynamic model offers a robust framework for predicting the melting temperature of cylindrical Ag nanoparticles, providing a crucial tool for researchers and engineers working to harness the unique properties of nanomaterials in innovative applications.

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