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Effect of shape and size on cohesive energy, Debye temperature and band gap of In_xSc_{1-x} Nanomaterial

Krishna Kumar[a], Mritunjay Kumar[a], Roma Kumari[a], Jagdhar Mandal[a*], Rupam Kumari[a]

[a] *University Department of Physics, TMBU Bhagalpur, Bihar*

[*] *Corresponding author: Email: jmandal1284@gmail.com*

Abstract

The study of nano-thermodynamic serves as a bridge between macroscopic and nanoscopic systems. A simple theoretical approach based on Qi and Wang model is used to investigate the shape and size dependent thermodynamic properties like cohesive energy, Debye temperature and energy band gap of In_xSc_{1-x} mixed nanomaterial. The cohesive energy has been used as an important thermodynamic quantity to explore the extent of effect of shape and size on important thermodynamic properties of In_xSc_{1-x} mixed nanomaterial. The properties of nanomaterial such as cohesive energy and Debye temperature decrease with decreasing size due to an increase in the number of dangling bonds in nanomaterials while band gap energy increases with decrease in size. They are also shape dependent. This mixed nanomaterial will then have device applications.

Keywords: *Mixed Nanomaterial, Nano-thermodynamics, Nanoscopic & Band gap energy, etc.*

Introduction

In the rapidly evolving field of nanoscience, nanomaterials have emerged as a fascinating class of materials whose properties defy traditional expectations [1-6]. At the nanoscale, where dimensions typically range from 1 to 100 nm, the interplay between shape and size becomes the key to unlocking a host of remarkable thermodynamic behaviors. The energy landscape of these materials is significantly altered by quantum confinement and the enhanced role of surface atoms, which in turn affects several fundamental properties. Among these properties, cohesive energy, Debye temperature and band gap energy all exhibit a strong dependence on the geometric configuration and size of the nanoparticles. Notably, the energy band gap is a crucial factor for electronic and optical applications can be precisely tuned in these systems, offering exciting possibilities for custom-designed nanodevices. Nanomaterials now have become the important link between nanoscience and nanotechnology.

To accurately capture these complex relationships, the Qi and Wang model [7-9] has been employed. This innovative framework builds on a myriad of earlier approaches, integrating insights from various models to predict how the thermodynamic parameters evolve as a function of both shape and size [10-17]. By focusing on the In_xSc_{1-x} system, researchers can explore a unique combination at the nanoscale, providing a rich platform for tailoring material properties through controlled compositional and morphological adjustments. The impact of these

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advancements is far-reaching, promising transformative applications [18-20] in areas ranging from catalysis and electronics to energy conversion and biomedical technologies. As we delve deeper into the thermodynamic intricacies of In_xSc_{1-x} nanomaterials, the Qi and Wang model [7-9] serves not only as a robust predictive tool but also as a testament to the power of integrating theory with experimental innovation in the quest for next-generation materials.

Formalism

The Qi and Wang model provides a theoretical framework to study the influence of nanoscale effects on the properties of mixed semiconductor compound nanomaterials. This model particularly focuses on size- and shape-dependent parameters, including cohesive energy, Debye temperature and energy band gap. These properties are critical for understanding and designing nanomaterials for advanced technological applications

Cohesive energy (E_{cn}): It is a measure of the energy required to disassemble a solid into its constituent atoms [21-22]. For mixed nanomaterials, the cohesive energy depends significantly on the surface-to-volume ratio. According to the Qi and Wang model, the cohesive energy, E_{cn} can be expressed as

$$E_{cn} = E_0 \left(1 - \frac{3N}{4n}\right) \quad (1)$$

Where as E_0 is cohesive energy of the bulk material per atom and n is the total number of atoms and N is the surface atoms.

For nanoparticles, $\frac{N}{n}$ is expressed in terms of shape and size parameter as

$$\frac{N}{n} = \alpha \frac{4d}{D}$$

then $$\frac{3N}{4n} = 3\alpha \frac{d}{D} \quad (2)$$

Where D represents the diameter of spherical nanoparticle, d represents atomic diameter and α denotes the shape parameter.

Therefore, from equations (1) and (2) the expression of cohesive energy of nanomaterial is expressed as

$$E_{cn} = E_0 \left(1 - 3\alpha \frac{d}{D}\right) \quad (3)$$

Debye temperature (θ_{DN}): It is a measure of the vibrational response of the nanomaterial atoms and this parameter reflects the binding forces between atoms and can be used to characterize the properties of many materials [23-26], such as thermal vibration and phase transition. According to Lindemann criterion [25] of melting, the Debye temperature θ_D is related to melting temperature T_m. The analytical expression for Debye temperature is given as

$$\theta_D = C \left(\frac{T_m}{MV^{2/3}}\right)^{1/2} \quad (4)$$

Where C is constant, M is the molecular mass and V molar volume. Equation (4) thus states that

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$\theta_D \propto (T_m)^{1/2}$

Likewise, the equation for Debye temperature of the nanomaterial can be written as

$$\theta_{DN} = C\left(\frac{T_m}{MV^{2/3}}\right)^{1/2} \quad (5)$$

Using the above relations in the expressions of Debye temperature for mixed nanomaterial is

$$\theta_{DN} = \theta_{DB}\left(1-\frac{3N}{4n}\right)^{1/2} = \theta_{DB}\left(1-3\alpha\frac{d}{D}\right)^{1/2} \quad (6)$$

Where, θ_{DN} and θ_{DB} are Debye temperatures in nanosolid and its counterpart bulk material respectively.

Energy Band gap (E_{gN}): The energy band gap (E_{gN}) determines the electronic and optical properties of semiconductors. For nanomaterials, the band gap widens as the size decreases due to the quantum confinement effect [27-30]. If the activation energy is equal to half of the relative change in energy bandgap in semiconductors. If E_{gN} and E_{gB} are energy bandgap in nanomaterial and its corresponding bulk material, the relative change in energy bandgap of nanomaterial is expressed as

$$\Delta E_{gN} = 2\,[E_a(B)] - [E_a(N)] \quad (7)$$

Therefore, the ratio of ΔE_{gN} to E_{gB} can be expressed as follows:

$$\frac{\Delta E_{gN}}{E_{gB}} = 1 - \frac{E_a(N)}{E_a(B)} = 1 - \frac{T_{mN}}{T_{mB}} \quad (8)$$

Where T_{mN} is melting temperature of nanomaterial and its corresponding bulk form is T_{mB}.

In view of expression (8), the expression for energy bandgap of nanomaterial in terms of shape and size parameter can be given as

$$E_{gN} = E_{gB}\left(1+\frac{3N}{4n}\right) = E_{gB}\left(1+3\alpha\frac{d}{D}\right) \quad (9)$$

This size dependency allows the fine-tuning of optical and electronic properties for specific applications, such as in quantum dots, optoelectronic devices, and photovoltaics.

Results and Discussion

The Qi and Wang model was applied to In_xSc_{1-x} nanomaterials to assess the influence of size and shape on key thermodynamic parameters such as cohesive energy (E_{cn}), Debye temperature (θ_{DN}) and energy band gap (E_{gN}). The model explains the variation of E_{cn}, θ_{DN} and E_{gN} for In_xSc_{1-x} nanostructured materials for concentration, (x=0.3). Therefore, we can easily verify our theoretical results by known experiment findings and results obtained by other co-workers. The model theory used in the present work requires shape parameters for different geometrics such as spherical nanosolids, regular tetrahedral, regular hexahedral, regular octahedral with their values 1, 1.49, 1.24 and 1.18 respectively. Atomic diameter of In_xSc_{1-x} is 0.2597 nm also used as input parameter.

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Using the atomic diameter and shape parameter as input the thermodynamic properties $E_{cn,}$ θ_{DN} and E_{gN} for different shape and size are calculated using the equations (3, 6 and 9) are used. The results are shown through the graphs marked as figures 1, 2 and 3. In these figures the computed results are compared with the results calculated from other theoretical researchers.

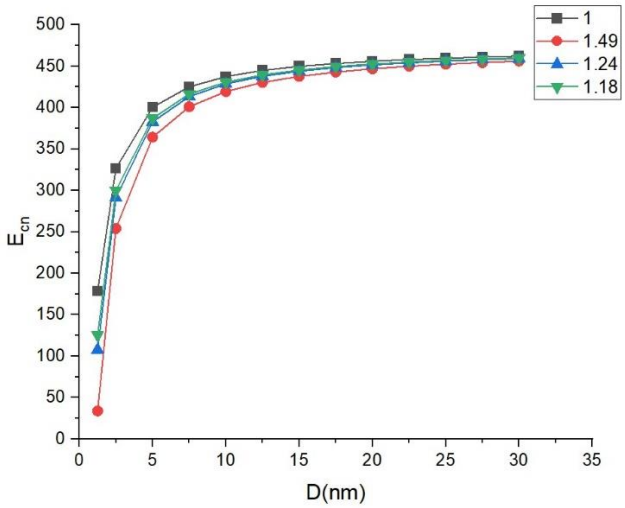

Figure 1: Shows the variation of E_{cn} (i.e., cohesive energy of nanomaterial) with size D (in nanometer) and shape parameter (α). The computed values for spherical, regular tetrahedral, regular hexahedral, regular & octahedral shape parameter (α) are shown by square(grey), circle(red) up triangle(blue) & down triangle(green).

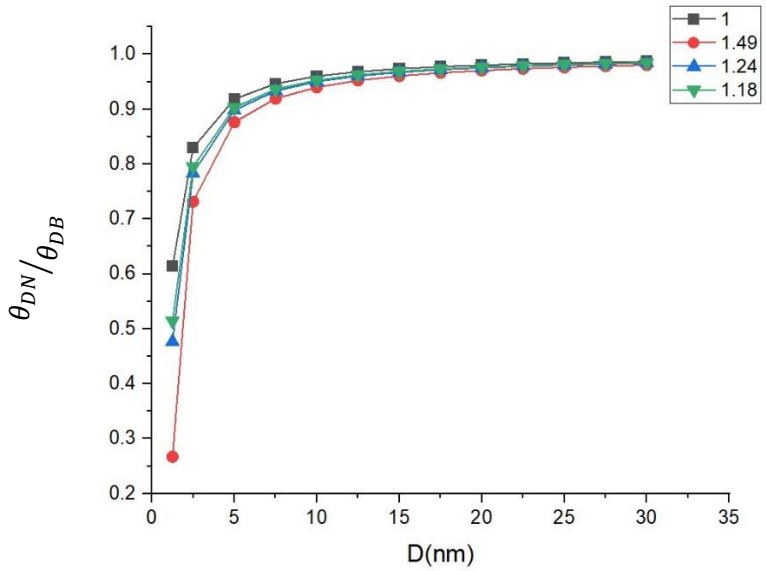

Figure 2: Shows the variation of θ_{DN}/θ_{DB} (i.e., Debye temperature of nanomaterial with respect to bulk material) with size D (in nanometer) and shape parameter (α). The computed values for spherical, regular tetrahedral, regular hexahedral, regular & octahedral shape parameter (α) are shown by square(grey), circle(red) up triangle(blue) & down triangle(green).

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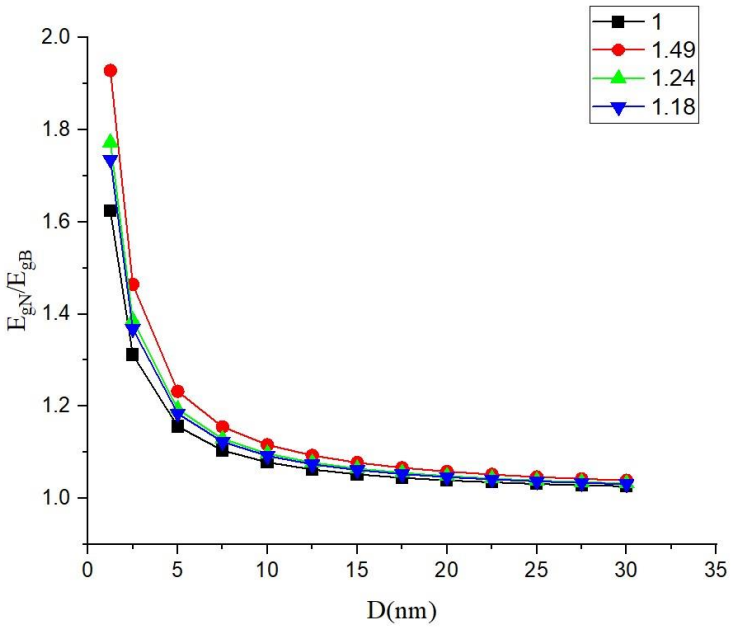

Figure 3: Shows the variation of E_{gN}/E_{gB} (i.e., band gap energy of nanomaterial with respect to the bulk material) with size D (in nanometer) and shape parameter (α). The computed values for spherical, regular tetrahedral, regular hexahedral, regular & octahedral shape parameter (α) are shown by square(grey), circle(red) up triangle(blue) & down triangle(green).

It is observed from figure 1 that the variation in cohesive energy is influenced by the shape and size [5]. This remains significant only when the nanomaterial size is below 20 nm. The cohesive energy shows an exponential increase up to 20 nm but beyond this point, the change is minimal and almost becomes stable. Thus, the cohesive energy in nanostructured mixture increases as grain size grows. It is known that the cohesive energy of the nanostructured material discloses the strength of the nanomaterial bond. Decreasing the cohesive energy of the nanomaterial means decreasing the nanomaterial bonds therefore, the nanomaterial bond is broken much easier, which consequently results in decreasing the melting point of the nanomaterials. When the particle size is larger than the 30 nm, the cohesive energy of the nanostructured materials In_xSc_{1-x} (x=0.3) are approximately equal to those of the corresponding bulk materials. The strong agreement between the present findings and those reported from experimental or other theoretical models confirms the accuracy and reliability of the model used.

Figure 2 illustrates the variation in the Debye temperature for In_xSc_{1-x} nano mixture compared to bulk materials as a function of particle size. The values, calculated using equation (6), and compared with results from Qi and Wang showing strong agreement with previous findings. The graphs reveal that the Debye temperature decreases non-linearly with the decrease in diameter(D) of the nanomaterials. The Debye temperature alters very slowly with the particle dimensions when the values of the diameter(D) are greater than 10 nm [23-24]. This behaviour is due to enhanced phonon confinement and surface effects in nanostructured materials. However, a **sharp decline** in Debye temperature is observed as the grain size approaches **5 nm**. Additionally, spherical nanosolids exhibit a **higher Debye temperature** than tetrahedral nanosolids of the same size, likely due to their more compact atomic

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arrangement and lower surface energy. Beyond **15 nm**, the impact of size and shape on Debye temperature becomes insignificant as the material transitions toward bulk-like behavior.

Figures 3 depicts the variation in energy bandgap of In_xSc_{1-x} nanomaterials with particle size and shape compared to bulk materials. The results are calculated using equation (9) with the Qi and Wang model. The band gap energy increases sharply as particle size decreases. It is observed that when the particle size is less than 6 nm there is a substantial increase in the band gap energy. This behaviour is expected to occur due to the fact that the holes in the balance band and the electrons in the conduction band are confined by the potential barriers of the surface [26-29]. However, beyond 10 nm, a decline is observed, indicating a transition where quantum effects weaken. Beyond 15 nm, the decrease stabilizes suggesting that the material approaches bulk-like behavior. The study also examines different nanostructured shapes, including spherical, tetrahedral, hexahedral, and octahedral geometries, showing minor variations but follows the same fundamental trend.

Conclusion

The present study employs the Qi and Wang model to comprehensively analyze the shape and size dependent thermodynamic properties of In_xSc_{1-x} nanomaterials. Our theoretical framework successfully quantifies the variations in cohesive energy, Debye temperature and energy band gap as a function of nanoparticle morphology. Key observations of the study are:

- A significant reduction in cohesive energy and Debye temperature with decreasing particle size reflecting weaker atomic interactions and increased surface effects.
- An increase in energy band gap as a consequence of quantum confinement and surface atom dominance.
- The pronounced effect of particle shape on these properties for sizes below 15–30 nm with the influence diminishing for larger nanocrystals.

These insights validate Qi and Wang model and also underscore its potential for guiding the design of nanomaterials with tailored thermophysical and optical properties. These properties pave the way for innovative applications in catalysis, optoelectronics, and energy conversion, offering a promising pathway for next-generation device technologies.

References:

1. Madan Singh, Monika Goyal, and Kamal Devlal, Journal of Taibah University of Science 12(4), 470-475, 2018.
2. M. Singh, BM Taele, and M. Goyal, Chinese Journal of Physics, 70 (2021) 26-36 https://doi.org/10.1016/j.cjph.2021.01.001
3. M. Goyal, B.R.K. Gupta, Mod. Phys. Lett. B 33 (2019) 1950310.
4. M. Goyal, B.R.K. Gupta, Pramana J Phys **90**(6), 80 (2018)
5. M. Goyal, B.R.K. Gupta, 47 (2018) 51–63.

DOI:10.5281/zenodo.15010195

6. M. Goyal and M. Singh, Applied Physics A (2020) 126:176, https://doi.org/10.1007/s00339-020-3327-9
7. W. H. Qi, Physica B, 368(2005) 46-50
8. W. H. Qi, M. P. Wang, Mater Chem Phys 88, 280 (2004)
9. W. H. Qi, M. P. Wang, Q. H. Liu, Journals of Material Science, 40(2005), 2737-2739.
10. Y. Qu, W. Liu, W. Zhang, C. Zhai, Phys. Met. Metall. 120 (2019) 417–421.
11. X. Liu, P. Yang, Q. Jiang, Mater. Chem. Phys., 103(2007) 1-7.
12. O. madelung, U. Roessler and M. Schulz, Landolt-Boerstein Substance/Property Index, vol. 41, pp. 1-16, 2002.
13. E. Steigmeier, Applied Physics Letters, vol. 3, no. 1, pp. 6-8, 1963.
14. A. Balerna and S. Mobilio, Physical Review B, vol. 34, no. 4, p. 2293, 1986.
15. A. I. Oliva and J. Lugo, 12th International Conference on Electrical engineering, Computing Science and Automatic control (CCE), 2015, pp. 1-6.
16. M. Omar, Advanced Materials Research, 2013, vol. 626, pp. 976-979.
17. A. K. Suleiman, Eurasian Journal of Science and Engineering 4, 19.
18. B. X. Wang, L. P. Zhou and X. F. Peng, International Journal of Thermophysics, vol. 27, no. 1, pp. 139-151, 2006.
19. L. Riviere, N. Causse, A. Lonjon, E. Dantras and C. Lacabanne, Polymer degradation and stability, vol. 127, pp. 98-104, 2016.
20. K. Kumar, M. Kumar, S. Ahmad, A. Kumar and J. Mandal, International Journal of Physics and Applications, 7(1), 2025, pp. 58-65.
21. H. C. Kopangkhotso, M. Singh and S. Singhal, International Journal of Advance Research in Science and Engineering, vol. 4, Issue (01), 2015, pp. 87-94.
22. M. Kumar, K. Kumar, S. Kumar, N. Kumari and J. Mandal, IJCSPUB (2025), vol. 15, pp. 722-731.
23. J. H. Rose, J. Ferrante and J. R. Smith, Physical Review Letters, vol. 47, no. 9, p. 675, 1981.
24. K. Nanda, S. Sahu and S. Behera, Physical review A, vol. 66, no. 1, p. 013208, 2002.
25. F. A. Lindemann, Phys. Z 11 (1990) 609.
26. J. M. Ziman, Cambridge University Press, Cambridge, 1976.
27. M. I. Ahamad, M. Ahamed, A. Sivaranjani and S. Chockalingam,
28. A. Kumar and K. Prasad, Nano Progress, 2021, 3(5), pp. 34-37.
29. Gregory Guisbiers, January 2012; Materials Research Society symposia proceedings. Materials Research Society 1371; DOI: 10.1557/opl.2012.
30. G. Guisbiers, Nano Express, 2010, 1132.

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