

Size and Shape Dependent Band Gap Engineering in III–V Nanosemiconductors Using Qi, Bond Energy and Guisbiers Models

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Abstract: In this study, the size- and shape-dependent variation of the energy band gap in III–V nanosemiconductors has been systematically investigated using three widely accepted phenomenological approaches, namely the Qi model, Bond Energy model, and Guisbiers model. The theoretical analysis has been performed for important III–V semiconductor compounds such as AlN, GaN, InN, GaAs, and InAs, considering different nanostructured geometries including spherical nanoparticles, cylindrical nanowires, and nanofilms. The band gap expansion (ΔE_g) has been evaluated as a function of particle size (diameter or width) as well as structural geometry. The obtained results clearly indicate that the energy band gap increases significantly with decreasing size of the nanostructures, which is mainly attributed to the quantum confinement effect arising from the spatial restriction of charge carriers at the nanoscale. It has also been observed that the geometry of the nanostructure plays an important role in determining the magnitude of band gap enhancement due to differences in surface-to-volume ratio. Among the models considered, the Guisbiers model provides the closest agreement with the available simulated and experimental data, demonstrating its superior predictive capability. Furthermore, the study examines the shifts in valence band and conduction band edges, revealing that the conduction band experiences a comparatively larger shift than the valence band. These findings offer a deeper understanding of size- and shape-controlled band gap engineering in nanostructured semiconductors and may be highly useful for the design and optimization of advanced optoelectronic, nanoelectronic, and photonic devices.

Keywords: Nanosemiconductors, Band Gap Expansion, Quantum Confinement, Guisbiers Model, Bond Energy Model, III–V Compounds.

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I. INTRODUCTION

Nanostructured semiconductors have received considerable attention in recent years because of their remarkable size-dependent electronic, optical, and structural properties, which differ significantly from those of bulk materials. When the dimensions of a semiconductor are reduced to the nanometer scale, the motion of electrons and holes becomes spatially confined. This phenomenon, known as quantum confinement, leads to substantial modification in the electronic band structure and results in an increase in the energy band gap[1-4]. Such size-induced changes make semiconductor nanostructures highly attractive for a wide range of technological applications[5].

Among various semiconductor materials, III–V compounds such as AlN, GaN, InN, GaAs, and InAs are of particular importance due to their excellent electrical and optical characteristics[16,18]. These materials are extensively used in advanced optoelectronic devices including light-

emitting diodes (LEDs), laser diodes, solar cells, photodetectors, and high-speed electronic components. Their tunable band gap properties at the nanoscale provide additional advantages for designing next-generation nanoelectronic and photonic devices.

The band gap of semiconductor nanostructures depends not only on particle size but also on shape and dimensionality. Spherical nanoparticles, cylindrical nanowires, and nanofilms exhibit different confinement strengths because of variations in their surface-to-volume ratio and geometrical symmetry[1-5,12]. Therefore, a systematic understanding of size- and shape-dependent band gap variation is essential for precise band gap engineering.

Several theoretical approaches have been developed to predict the variation of band gap in nanomaterials. Among them, the Qi model, Bond Energy model, and Guisbiers model are widely recognized because of their simplicity, fewer input parameters, and reliable predictions. In the

present work, a comparative analysis of these three models has been carried out to investigate band gap expansion in different III–V semiconductor nanostructures[6-11,19].

II. THEORETICAL BACKGROUND

The variation of energy band gap in semiconductor nanostructures has been explained through several theoretical and phenomenological models. These models are useful for predicting the dependence of band gap on particle size, dimensionality, and structural geometry. In the present study, three widely used approaches, namely the Qi model, Bond Energy model, and Guisbiers model, have been employed to analyze the size- and shape-dependent band gap expansion in III–V nanosemiconductors.

➤ *Qi Model*

The Qi model is one of the commonly used phenomenological models for describing the band gap expansion in semiconductor nanoparticles. This model assumes that the band gap energy changes with particle size because of the increased influence of surface atoms when the dimensions are reduced to the nanoscale. The model uses basic material parameters such as atomic diameter and bulk band gap energy as input quantities. Due to its simple mathematical form and limited number of parameters, the Qi model is widely used for estimating size-dependent band gap changes in nanoscale systems[8,9].

➤ *Bond Energy Model*

The Bond Energy model is an extension of the Qi model and provides a more flexible approach for analyzing nanoscale band gap variation. In this model, a relaxation factor (δ) is introduced to account for bond contraction and bond energy changes at the surface of the nanomaterial. Since surface atoms experience a different bonding environment compared to bulk atoms, their contribution becomes significant at smaller sizes. The Bond Energy model can therefore predict band gap variation more accurately for certain nanostructures. For the specific case of $\delta = 1/2$, the Bond Energy model reduces exactly to the Qi model[10,11].

➤ *Guisbiers Model*

The Guisbiers model further improves the prediction of band gap variation by incorporating the effect of nanostructure geometry through a shape-dependent parameter (α_{shape}). Since spherical nanoparticles, cylindrical nanowires, and nanofilms possess different surface-to-volume ratios, their quantum confinement behavior differs significantly. By including the shape parameter, the Guisbiers model becomes more suitable for analyzing band gap expansion in nanostructures of various geometries and dimensions. This model often provides better agreement with experimental and simulated results[6,7].

III. METHODOLOGY

In the present study, the size- and shape-dependent band gap expansion (ΔE_g) of III–V semiconductor nanostructures has been evaluated using the Qi model, Bond Energy model, and Guisbiers model. The calculations have been carried out for different nanoscale geometries in order to investigate the influence of dimensionality and morphology on the electronic properties of the materials. Three major forms of nanostructures have been considered: spherical nanoparticles (quantum dots), cylindrical nanowires, and nanofilms. These structures represent zero-dimensional, one-dimensional, and two-dimensional confinement systems, respectively, and therefore exhibit different quantum confinement effects[6,11].

The required input parameters for the theoretical calculations include the atomic diameter (d), bulk band gap energy (E_g^B), and shape-dependent parameter (α_{shape}). The atomic diameter is used to account for the characteristic atomic dimensions of the semiconductor compound, while the bulk band gap energy represents the intrinsic band gap of the corresponding bulk material. The shape parameter is particularly important in the Guisbiers model, where the geometry of the nanostructure influences the surface-to-volume ratio and consequently the magnitude of band gap expansion[6,7].

To compare the effect of geometry, a form factor ratio has been adopted for different nanostructures. The values are taken as 3 for spherical nanoparticles, 2 for cylindrical nanowires, and 1 for nanofilms. These ratios indicate the relative degree of confinement and available surface area for each structure. Spherical nanoparticles possess the highest confinement in all three dimensions, while nanofilms show confinement mainly in one dimension[6].

Using these input parameters, the band gap expansion has been calculated as a function of particle diameter or film width for AlN, GaN, InN, GaAs, and InAs nanosemiconductors. The obtained results from the three models are then compared to examine their suitability and predictive accuracy for different nanostructured systems[6,8-11].

IV. RESULTS AND DISCUSSION

➤ *Size Dependence of Band Gap*

The calculated results clearly demonstrate that the energy band gap increases with decreasing size for all considered nanostructures[1-5,12]. This behavior has been consistently observed for AlN, GaN, InN, GaAs, and InAs compounds in the form of spherical nanoparticles, cylindrical nanowires, and nanofilms[6-11,16,17]. The increase in band gap becomes more significant at smaller particle dimensions, particularly below approximately 10 nm, where quantum confinement effects become dominant. As the particle size approaches the excitonic Bohr radius, the motion of electrons and holes becomes spatially restricted, resulting in widening of the forbidden energy gap.

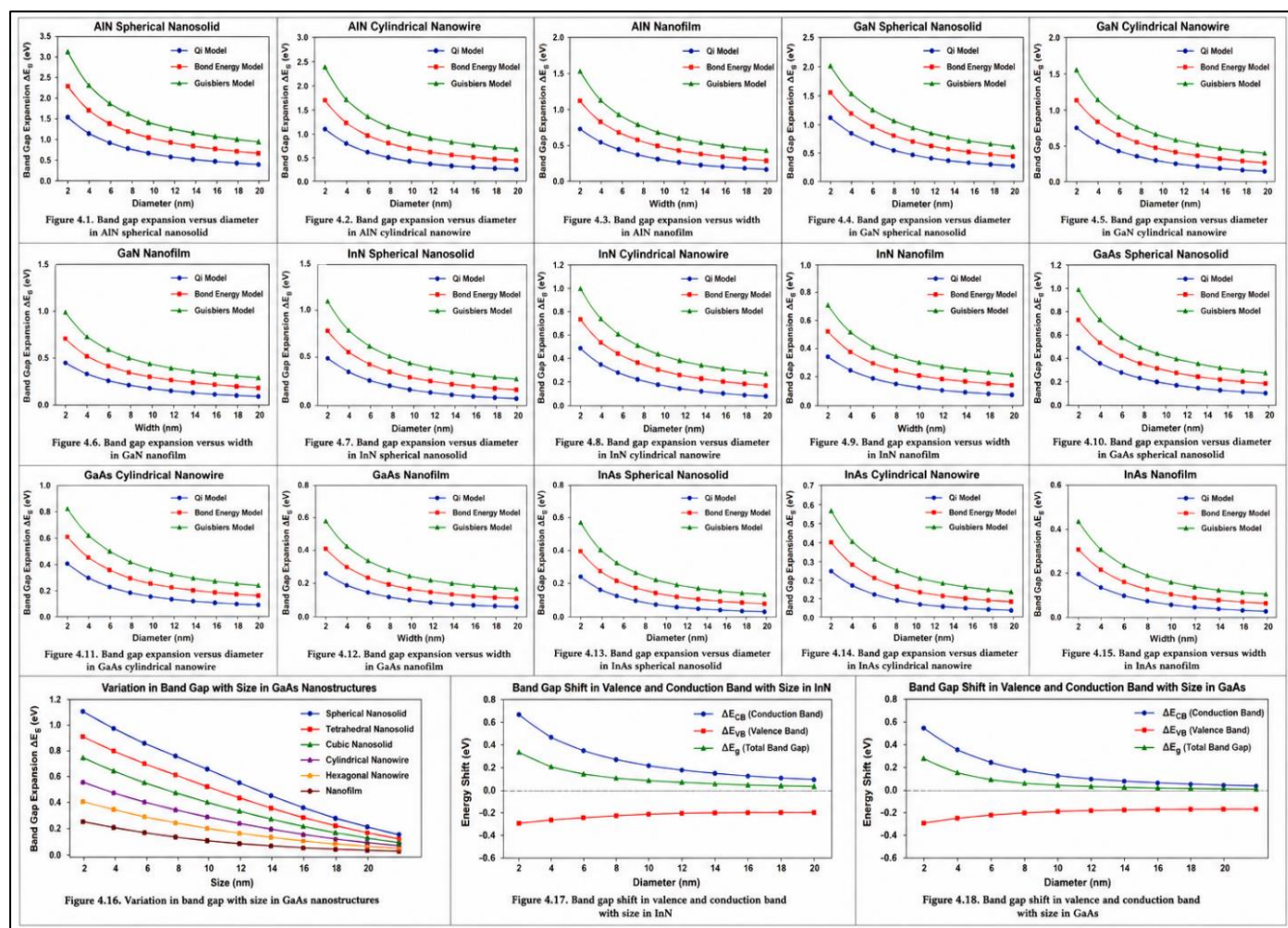


Fig 1 Size Dependence of Band Gap

For AlN nanostructures, the variation of band gap with size for spherical nanoparticles, cylindrical nanowires, and nanofilms is shown in Figure 1, Figure 2, and Figure 3, respectively. Similarly, the corresponding results for GaN are presented in Figure 4, Figure 5, and Figure 6. In the case of InN, the size-dependent band gap expansion is illustrated in Figure 7, Figure 8, and Figure 9. For GaAs nanostructures, the results are shown in Figure 10, Figure 11, and Figure 12, while those for InAs are presented in Figure 13, Figure 14, and Figure 15.

➤ Shape Dependence

The obtained results reveal that band gap expansion strongly depends on the geometry of the nanostructure. Among the considered shapes, spherical nanoparticles exhibit the maximum increase in band gap due to confinement in all three dimensions. Cylindrical nanowires show moderate enhancement, whereas nanofilms display the minimum band gap shift because confinement occurs mainly in one dimension. This trend is directly related to differences in surface-to-volume ratio and carrier confinement strength[6,7,10].

The comparative variation of band gap for different GaAs nanostructure geometries such as spherical, tetrahedral,

cubic nanoparticles, cylindrical and hexagonal nanowires, and nanofilms is illustrated in Figure 16.

➤ Model Comparison

A comparison of the three theoretical models indicates that the Guisbiers model provides the best agreement with available simulated and experimental data for almost all semiconductor compounds and geometries. The Bond Energy model also gives reliable predictions for suitable values of relaxation factor (δ), while the Qi model serves as a basic approximation for size-dependent band gap variation. Therefore, the Guisbiers model is found to be the most reliable and effective model for predicting band gap expansion in nano semiconductors[6-11].

➤ Material-Wise Analysis

For AlN, GaN, and InN, which crystallize in the Wurtzite structure, strong band gap enhancement is observed with decreasing size[16,17]. The predicted values show good agreement with theoretical and available experimental results. In contrast, GaAs and InAs, having Zinc-Blende crystal structure, also exhibit clear size dependence, with better model prediction particularly at smaller nanostructure sizes[17,18].

➤ Band Edge Shift (VB and CB)

The variation of valence band (VB) and conduction band (CB) edges with size has also been analyzed. It is observed that the conduction band shift (ΔE_{CB}) is greater than the valence band shift (ΔE_{VB}). Both edges move as the nanostructure size decreases, leading to an overall increase in band gap energy. This behavior is a direct consequence of quantum confinement effects[3,4,12,15].

The band edge shifts for InN and GaAs nanostructures are shown in Figure 17 and Figure 18, respectively.

➤ Physical Explanation

The increase in band gap with decreasing size is mainly attributed to quantum confinement, carrier localization, and enhancement in surface-to-volume ratio. As the dimensions of the semiconductor decrease, discrete energy levels begin to form, causing the optical transition to shift toward higher energy. This phenomenon is commonly known as the blue shift[1-4,12,19].

V. CONCLUSION

This study presents a comprehensive theoretical analysis of band gap expansion in III–V nanosemiconductors using the Qi model, Bond Energy model, and Guisbiers model. The results confirm that the band gap increases significantly with decreasing size and strongly depends on the shape of the nanostructure. Spherical nanoparticles exhibit the highest confinement effect, while nanofilms show the least. Among the considered models, the Guisbiers model provides the most accurate predictions. Furthermore, the conduction band shift is found to dominate over the valence band shift. These findings are highly useful for the design and optimization of nanoscale optoelectronic and nanoelectronic devices[6-12,16-19].

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