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رابح بونار

Band gap energies and optical properties in nanostructured semiconductor InAs: The Effect of Quantum Confinement

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Abstract

In the zinc-blende phase, the impact of quantum confinement on the band gap energies and refractive index of spherical semiconductor nanostructured InAs has been examined. Utilizing a pseudopotential approach, this study emphasizes the connection between the electronic and optical properties and the size of quantum dots. The results indicate that quantum confinement results in a significantly larger fundamental energy gap, whereas the refractive index decreases notably. This study underscores the influence of quantum confinement on the electronic properties of semiconductor quantum dots and their potential for various technological applications.

Keywords: *Band gap energy; Optical properties; InAs semiconductors; Quantum dots.*

1. Introduction

Indium arsenide (InAs) is a semiconductor material made up of indium (In) and arsenide (As), known for its direct band gap. Most experimental assessments of its energy gaps at low temperatures range from 0.41 to 0.42 eV [1]. In recent research by Lacroix et al. [2], a high-purity InAs sample was used to distinguish between shallow impurity, exciton, and band-to-band transitions, resulting in a reported value of 0.417 eV. At room temperature, the direct band-gap energy is generally suggested to be 0.36 eV [3,4]. InAs is distinguished by its narrow energy band gap and high electron mobility, appearing as grey crystals with a cubic structure. It is employed in the development of infrared detectors for wavelengths between 1 and 3.8 μm and

acts as the electron quantum well material in InAs/GaSb/AlSb-based electronic devices [5]. The fundamental characteristics of bulk InAs are well-documented with high accuracy [1].

However, the emerging class of materials formed by semiconductor nanostructures offers a largely unexplored range of potential applications. Nanoscale materials such as semiconductor quantum dots display electronic and optical properties that fall between those of larger macro- and microscale bulk semiconductor crystals and much smaller atoms and molecules [6]. Since the nanoscale is comparable to the Bohr exciton radius of electron-hole pairs in solids, semiconductor quantum dots display quantum size effects, particularly those associated with quantum mechanical particles in a three-dimensional box [7]. Quantum dots can be created in a monolayer of InAs on InP or GaAs. The differences in lattice constants between these materials induce surface layer tensions, which subsequently result in the formation of quantum dots. Additionally, quantum dots can be formed in InGaAs, with InAs dots embedded in the GaAs matrix [8]. These have been produced with peak optical emission wavelengths spanning from the ultraviolet to the visible and into the infrared spectrum. In this study, the electronic and optical properties of InAs spherical quantum dots have been examined. The objective of this paper is to discover new electronic and optical properties that are unattainable in unconfined (bulk) InAs compound semiconductors. The calculations primarily rely on the empirical pseudopotential method (EPM). The EPM, even at the nanoscale, has been demonstrated to yield accurate results [9,10]. Moreover, the computational effort required by this method is significantly less than that needed for first-principles calculations

2. Computational details

As noted in the literature, particularly in Ref. [11], the local empirical pseudopotential approach is widely recognized. For bulk InAs, the pseudopotential Hamiltonian for an electron within the crystal is composed of a kinetic-energy component along with a weak potential that is dependent on:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \quad (1)$$

The potential V can be represented as an expansion in terms of reciprocal lattice vectors G, and it is described as the product of a structure factor S(G) and a pseudopotential form factor VG. The bulk eigenfunctions ϕn,k are solutions to the time-independent Schrödinger equation,

$H\phi_{n,k} = E_{n,k}\phi_{n,k}$ (2)

are expanded in terms of a linear combination of plane waves. For a binary In cases like this, the expansion is divided into two components: one symmetric and the other antisymmetric, relative to the exchange of two atoms around their midpoints. We address the Schrödinger equation by finding the roots of the secular equation, which is derived from the Hamiltonian matrix. The zinc-blende matrix is intricate because the matrix elements of the antisymmetric potential are imaginary. Applying the EPM to compute the band structure properties of quantum dots necessitates reducing the electron's environment from a three-dimensional bulk to a zero-dimensional quantum dot. Here, dimensionality pertains to the number of degrees of freedom in electron momentum. The reduced dimensionality in semiconducting quantum dots often leads to the discretization of energy states, resulting in molecular-like orbital energies instead of a band structure [13]. These energy levels are determined by applying appropriate boundary conditions to the wave functions. In this study, the allowed k values have been derived by refining boundary conditions that depend on the shape and size of the dots, specifically for spherical quantum dots. We ascertain the form factors by aligning the atomic form factors, treated as adjustable parameters, with experimental data. Adjustments to the specific pseudopotential form factors are made using a non-linear least-squares fitting method [4,12]. In this paper, the experimental band-gap energies for bulk InAs at the Γ, X, and L high-symmetry points in the Brillouin zone, fixed in the fits, are 0.36, 1.37, and 1.07 eV [3], respectively.

3. Results and discussion

Figure 1 illustrates how the direct (Γ–Γ) band-gap energy varies with the diameter of zinc-blende InAs spherical quantum dots, specifically within the 1–3 nm range. It is observed that as the quantum dot's radius expands from 1 to 3 nm, the direct band gap (Γ–Γ) diminishes swiftly and consistently. Previous studies on nanostructured GaAs [17] and GaN spherical quantum dots [18] have shown that once the size exceeds 3 nm, the reduction in the direct band gap (Γ–Γ) becomes less pronounced and starts to approach the bulk value. Therefore, a similar trend is anticipated for the direct band gap (Γ–Γ) in InAs quantum dots when their size surpasses 3 nm.

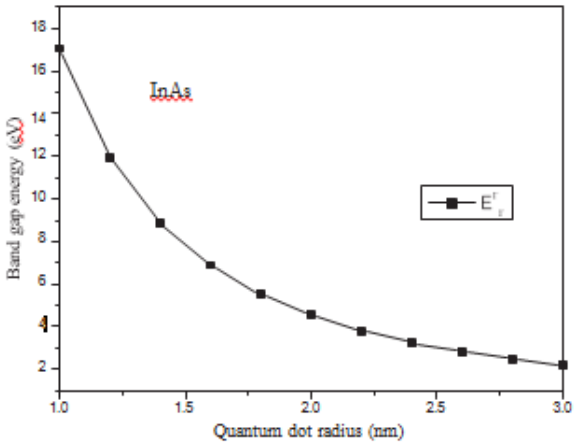

Fig. 1. Direct band gap (Γ–Γ) in nanosized InAs versus quantum dot radius.

The quantum confinement effect is responsible for opening the (Γ–Γ) direct band gap when the radius is less than 3 nm. As a result, the direct (Γ–Γ) band-gap energy, influenced by quantum confinement, becomes significantly larger than the unconfined or bulk band-gap energy. In a quantum dot with a size comparable to the exciton Bohr radius, the electron and hole forming an exciton are influenced by the dielectric boundary, which strongly affects their movements. However, if the quantum dot is much larger than this scale, the dielectric confinement effect is minimal, making the situation similar to that in a bulk medium. The direct (Γ–Γ) band gap for bulk, as determined in this study, is 0.36 eV, which aligns well with the experimental values cited in Refs. [3,4]. Regarding the direct (Γ–Γ) band-gap energies for InAs quantum dots, our findings are predictions due to the absence of experimental and theoretical data in the literature, as far as we know. The refractive index of semiconducting materials is a crucial physical property that defines their optical characteristics [19]. Moreover, devices like photonic crystals, waveguides, solar cells, and detectors require prior knowledge. The refractive index for spherical quantum dots has been calculated as a function of quantum dot radius in the range of 1–3 nm using various models, all directly related to the fundamental energy bandgap (Eg). Our results are illustrated in Fig. 2. We note that for all models used, the refractive index for InAs quantum dots increases rapidly as the quantum dot radius grows from 1 to 3 nm, showing a monotonic behavior. The bulk InAs refractive index is determined to be 3.75 using the Hervé and Vandamme empirical relation [23], which is consistent with the commonly reported value of 3.51 in Ref. [24].

Therefore, the predicted refractive index for InAs quantum dots with a nanocrystal diameter between 1–3 nm is found to be significantly lower than the bulk value for all models used in this study. Our refractive index data are fitted using a least-squares method, resulting in the following analytical expressions that relate the refractive index to the quantum dots radius a as,

$$n(a) = 1.95 + 0.77a - 0.14a^2 \quad \text{(Moss model)} \quad (3)$$

$$n(a) = 1.46 + 1.41a - 0.27a^2 \quad \text{(Gupta and Ravindra model)} \quad (4)$$

$$n(a) = 1.74 + 0.99a - 0.18a^2 \quad \text{(Hervé and Vandamme model)} \quad (5)$$

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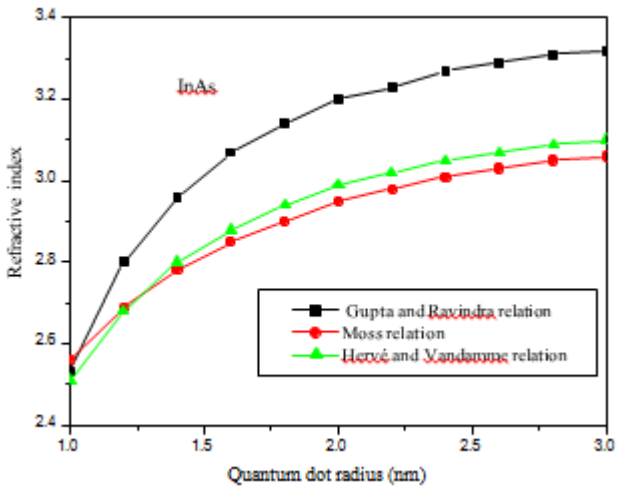

Fig. 2. Refractive index in nanosized InAs versus quantum dot radius using different models

4. Conclusion

In conclusion, this study examined how the electronic and optical properties of zinc-blende InAs spherical quantum dots vary with quantum dot radius. Key parameters, including the direct band-gap energy and refractive index, were evaluated for quantum dots with radii ranging from 1 to 3 nm using the empirical pseudopotential method. The calculated results for bulk InAs demonstrated strong agreement with previously reported data. Furthermore, quantum confinement was shown to play a significant role in determining these properties, leading to a

widening of the direct band gap and a notable reduction in the refractive index compared to the corresponding bulk values.

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