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Polarization-dependent intervalence band absorption in quantum dots

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Abstract

In this work, we compute the electronic band structure of ZnCdSe/ZnS semiconductor quantum dots (QDs) using *k. p* method, and studied the dependence of QDs parameters on the in-plane polarization anisotropy and degree of polarization (DOP) of intersubband absorption spectra of QDs. Higher energy levels in the valence band show nonlinear dependence on the parabolic confinement strength and exhibit strong anti-crossing. We find that the optical transitions for specific polarization directions are defined by the size, strain, and shape anisotropy of the QDs. We observe that increasing the shape anisotropy, strain, and QDs radius enhanced the in-plane polarization anisotropy, whereas increasing QDs height reduces the in-plane polarization anisotropy. The DOP is found to increase with increasing QDs radius and strain and reducing the shape anisotropy and QDs height. Furthermore, the QDs parameters play a key role in deciding the absorption peak of the

specific polarization. The present study suggests that the combination of shape, size, and strain could provide an optimal approach to tune the intraband polarization response from QDs.

Introduction

The semiconductor quantum dots (QDs) have revolutionized the prospects of the modern era of science and technology, including photonics, electronics, and medical technologies, due to their appealing electronic and optical properties, which are significantly different from those of their bulk counterparts [[1], [2], [3]]. The three-dimensional (3-D) quantum confinement caused by the surrounding wide band gap barrier materials, which results in the discretization of energy states and the δ-function-like density of states, yields many fascinating properties, including a lower threshold current, high-temperature operation, better radiation hardness, enhanced stability, and so on [[4], [5], [6], [7]]. Moreover, the properties of quantum dots and their possible applications significantly depend on the method by which they have been obtained. Further, their properties can be tuned in a controllable way by changing the geometry of the structure and externally applied magnetic and electric fields [[8], [9], [10]].

In recent years, QDs have been extensively explored to develop mid- and far-infrared optical sources and detectors, which are expected to enable a myriad of applications, covering chemical spectroscopy, pollution monitoring, thermal imaging, remote sensing, and biological imaging [[11], [12], [13], [14], [15], [16]]. Unlike the interband transitions between the conduction and valence bands, the QDs utilize intraband transitions among the sub-bands within the conduction or valence band to access the infrared spectral window. The group III-V compound semiconductors based matured QDs have been the dominant materials system investigated for the intraband QDs devices. Nonetheless, II-VI QDs have recently been extensively investigated for their potential in intraband QD devices [[17], [18], [19]]. More importantly, II-VI QDs can be grown using the chemical route without requiring high-end, sophisticated instruments [[20], [21], [22]]. QDs grown using such a technique are well recognized as colloidal QDs. Intraband transitions in these colloidal QDs have been promising for cost-effective mid- and far-infrared optical sources and detectors.

While the intersubband transitions in the QDs have been widely reported in the literature [[23], [24], [25], [26]]. However, polarization-dependent research is scarce. Therefore, we investigate the polarization-dependent intraband transitions occurring within the various valence band energy levels in the QDs. The ZnCdSe/ZnS QDs system has been intentionally chosen for the investigation because of the large valence band offset between ZnCdSe and ZnS barrier, which allows the accommodation of a sufficient number of holes and, thus, covers a broad spectral range. Additionally, holes, having a larger effective mass than electrons as charge carriers, suppress tunneling and permit the design of devices with thinner barrier layers.

To compute the electronic structure of QDs, various theoretical models such as the tight binding approach, the Hubbard model, the pseudopotential method, and the multiband k. p approach are widely used [27,28]. Among these, the multiband k. p approach provides better computational efficiency as well as reasonable accuracy and takes into account valence-band degeneracy, allowing for a better description of the valence band [29]. Furthermore, it is particular useful for describing the electronic structure of direct gap semiconductor near the band edges [30]. Therefore, we apply a multiband **k. p** approach based on the standard Kohn-Luttinger Hamiltonian to compute the

electronic structure of the ZnCdSe/ZnS QDs. After that, we evaluate the optical transitions and absorption spectra between the various valence band sub levels. Valence band mixing and strain effects have been taken into account to describe the polarization-dependent intraband optical transitions. We have shown that shape anisotropy, and QD dimension might be effective tools to tailor the intraband polarization behaviour of the QDs.

Section snippets

Theoretical formulation

The study of electronic and optical properties of QDs requires proper treatment of the semiconductor band structure. While analysing the electronic behaviour critically, the valence band in semiconductors cannot be approximated by a simple single parabolic band model since it consists of degenerate heavy, light, and split-off hole subbands [31,32]. Quantum confinement and strain-induced effects reduce this degeneracy. Finite optical transitions can occur between any of these subbands, and there …

Results and discussion

The material parameters used in this analysis are given in Table 1. We use the valence band offset between CdSe and ZnS=0.60eV, and between ZnSe and ZnS=0.53eV, according to reference [41]. We use σ=20meV, which is close to the value found in these dots. The band gap for the $Zn_{1-x}Cd_xSe$ is determined as $Eg(x)=E_{gCdSe}+(E_{gZnSe}-E_{gCdSe}-b_o)x+b_ox^2$, where b_o represents bowing parameter with value=0.301 [42]. All other parameters for $Zn_{1-x}Cd_xSe$ were determined using a linear …

Conclusions

The study aimed to find a practical approach to tune the intraband polarization response from QDs. We have studied the impact of size, strain, and shape of QDs on the polarization features of the absorption spectra. A study of the hole energy levels unfolds that the excited states exhibit nonlinear dependence on the in-plane parabolic confinement strength ($\hbar\omega_0$) while the ground state varies linearly with the $\hbar\omega_0$. We find the profound effect of QD radius on the polarization-dependent absorption …

Authors' contributions

Kiran Rathi conducted the theoretical analysis and provided the results.

Saral K. Gupta provided the ideas and structure of the whole article.

Jitendra Kumar interpreted the results and provided the "Results and discussion" section of the article.

C. M. S. Negi wrote the whole article. All authors read and approved the final manuscript. …

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. …

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