

Characterizing and Modelling Quantum Dashes for InP-Based Semiconductor Lasers

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Finally, thank you and much love to my family, who help me keep things in perspective. To Pa, chardi kala.

Abstract

InAs/InP multiwavelength quantum dash lasers are promising solutions to rising data loads in our telecommunications systems, as one laser chip can replace many lasers operating at a single wavelength [1]. Quantum dashes are quasi-one-dimensional nanoparticles that offer equal or increased performance as laser gain media when compared to equivalent quantum well devices [2], [3]. InAs/InP quantum dashes are ideal for laser devices emitting in the C-band region, centred around 1550 nm. The quantum dashes in this thesis are epitaxially grown via the self-assembled Stranski-Krastanow mode.

Characterizing how structure and composition of these quantum dashes affect the energy level spacing and emission wavelengths is crucial for designing better performing telecommunications lasers. In this thesis a method for determining the average heights and widths of these nanoparticles from atomic force microscopy measurements of uncapped InAs/InGaAsP/InP quantum dashes is developed. Single quantum dash simulations are built in Crosslight Photonic Integrated Circuit Simulator (PICS3D) with the lowest energy transition tuned to photoluminescence peak wavelengths provided by National Research Council Canada. These simulations are used to determine the impact of quantum dash dimensions, compositions, and heterostructure changes to the overlap integrals and emission energies.

Phosphorus concentration within the quantum dash and wetting layer can modify the predicted emission wavelength by ~ 200 nm, and increasing quantum dash lengths beyond 200 nm has negligible effect on emission energy and energy level spacing. The sublayer thickness is increased from 0.1 to 1 nm, and shows that emission energy will increase for GaP sublayers and decrease for GaAs sublayers by up to 30 meV. The role of the wetting layer on energy level spacing is discussed and determined to increase the emission energy by ~ 15 meV when the 0.5 nm wetting layer is removed for a 2 nm quantum dash. The role of As/P intermixing is investigated in three ways: by incorporating phosphorus concentration in (1) the quantum dash and wetting layer, (2) the wetting layer, and (3) the lower portion of the quantum dash without a wetting layer. There is negligible change in the overlap integral for these three cases with all other variables held constant, and the trends between each case remain the same.

Further experimental analysis of buried InAs quantum dashes is recommended for compositional information. The implementation of variable strain profiles in this model is also recommended, in addition to developing vertically coupled quantum dash simulations. Finally, performing these simulations at varying temperatures will better represent the operating conditions of quantum dash lasers.

Contents

1	Introduction	1
1.1	History and Background	2
1.2	Motivation and Structure	3
2	Theory and Background	5
2.1	Band Structure and Single Band Parabolic Model	5
2.1.1	Zinc-Blende Semiconductors	6
2.1.2	Valence Band Splitting and Strain	7
2.1.3	Quantum Confinement	10
2.1.4	Band Alignment	11
2.2	Density of States	12
2.2.1	Ideal Density of States Derivations	13
2.3	Electron Transition Rules	16
2.3.1	Scattering Processes	16
2.3.2	Fermi's Golden Rule	17
2.4	Self-Assembly of InAs/InP Nanoparticles	19
3	Experimental Methods	23
3.1	Nanoparticle Growth	23
3.1.1	Chemical Beam Epitaxy	23
3.1.2	Sample Descriptions	23
3.2	Atomic Force Microscopy	25
3.2.1	Procedure for AFM Image Acquisition	25
3.2.2	Procedure for Post-Processing of AFM Images	26
3.3	Energy Level Simulations	28
3.3.1	Description of Model	28
3.3.2	Simulation Setup and Mesh Convergence	31

4 Atomic Force Microscopy Experiments	34
4.1 Overview	34
4.2 Preface and Author Contributions	35
4.3 Publication - Photonics West 2022	36
5 Single Quantum Dash Simulations	43
5.1 Preface and Author Contributions	43
5.2 Publication - Submitted November 2022	43
6 Effect of Wetting Layer on Emission Energy and Overlap Integrals	51
6.1 Effect of Wetting Layer on Emission Energies	51
6.1.1 QDash Height and the Wetting Layer	52
6.1.2 Phosphorus Concentration and the Wetting Layer	53
6.2 Overlap Integrals and Mode Confinement	56
7 Conclusions	60
7.1 Further Research	60
7.2 Conclusion	60
8 Appendix	62
8.1 Processed AFM images	62
8.2 AFM Data Processing	64
8.2.1 AFM Height Distributions of $1\ \mu\text{m}^2$ AFM images	64
8.3 Crosslight Simulation Code	65
8.3.1 Layer Files	65
8.3.2 Solution File box.sol for 1.5nm QDash	72
8.3.3 Output File box.qdd and Processing	73
8.4 k·p Method for Determining Band Structure	83
8.4.1 General k·p Theory and Background	83
8.4.2 4×4 k·p Theory	85
References	87

List of publications and contributions

This thesis begins with an introduction to quantum confinement and nanoparticles, and then presents two publications by the author. The first describes the atomic force microscopy measurements and analysis process of uncapped InAs/InGaAsP/InP nanoparticles, published through the SPIE Photonics West 2022 Conference Proceedings. The second is a manuscript submitted to Applied Physics Letters containing single quantum dash simulation results. Further simulation results are shown in Chapter 6.

1. **Ras-Jeevan K. Obhi**, Sebastian W. Schaefer, Christopher E. Valdivia, Philip J. Poole, Jiaren Liu, Zhenguo Lu, and Karin Hinzer, "Height distributions of uncapped InAs/InGaAsP/InP quantum dashes and their effect on emission wavelengths," Proc. SPIE 12010, Photonics and Phononic Properties of Engineered Nanostructures XII, 120100C (5 March 2022); doi: 10.1117/12.2609954.
2. **Ras-Jeevan K. Obhi**, Sebastian W. Schaefer, Christopher E. Valdivia, Jiaren Liu, Zhenguo Lu, Philip J. Poole, and Karin Hinzer, "Indium arsenide single quantum dash morphology and composition for wavelength tuning in quantum dash lasers", submitted November 2022 to Applied Physics Letters (APL).

The author also contributed to the following works throughout their graduate studies.

1. **Ras-Jeevan K. Obhi**, Sebastian W. Schaefer, Christopher E. Valdivia, Philip J. Poole, Jiaren Liu, and Karin Hinzer, "Effect of phosphorus concentration on the emission wavelength of InAs/InGaAsP/InP quantum dashes", Photonics West 2022 Poster + Online Presentation (PW On-Demand), Feb 2022, Permanent url: <http://hdl.handle.net/10393/43518>
2. **Ras-Jeevan K. Obhi**, Erin M. Tonita, Mandy R. Lewis, Christopher E. Valdivia, Mariana I. Bertoni, and Karin Hinzer, "Angle dependent quantum efficiency measurements of bifacial silicon solar cells", Photonics North 2020 Abstract and Express Presentation, May 2020.
3. Sebastian W. Schaefer, **Ras-Jeevan K. Obhi**, Christopher E. Valdivia, Philip J. Poole, Jiaren Liu, Zhenguo Lu, Pedro J. Barrios, and Karin Hinzer, "Effect of temperature on internal efficiency in InGaAsP/InP quantum dash lasers", Photonics West 2022 Online Presentation (PW On-Demand), Feb 2022.

4. Sebastian W. Schaefer, **Ras-Jeevan K. Obhi**, Christopher E. Valdivia, and Karin Hinzer, "Effect of Wetting Layers on Quantum Dash Laser Operation in Crosslight PICS3D", NUSOD 2021 Presentation.
5. Sebastian W. Schaefer, **Ras-Jeevan K. Obhi**, Christopher E. Valdivia, and Karin Hinzer, Philip J. Poole, Jiaren Liu, and Zhenguo Lu, "Quantifying Loss Mechanisms in In-GaAsP/InP Quantum Dash and Quantum Well Lasers", Photonics North 2021 Presentation.

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Declaration of Originality

The work contained in this thesis was performed and written by Ras-Jeevan K. Obhi with contributions by co-authors as outlined, under the supervision of Professor Karin Hinzer. To the best of the author's knowledge, these results are original.

List of Figures

2.1	General simplified bandgap diagrams in real and momentum space	6
2.2	Binary zincblende III-IV semiconductors with lattice constants	7
2.3	Compressive and tensile strained lattices	9
2.4	General picture of band structure	10
2.5	Bulk vs. quantum heterostructures	11
2.6	Band alignments for heterostructures	12
2.7	Ideal density of states summary	13
2.8	Scattering processes in a laser gain medium	17
2.9	Types of epitaxial thin layer growth	20
3.1	Description of nanoparticle samples	24
3.2	Flowchart mapping Crosslight simulation process	29
3.3	Simulation structure in multiple views	30
3.4	Visual description of Crosslight mesh parameters	32
3.5	Established x - y mesh for single quantum dash simulations	33
3.6	Established z mesh for single quantum dash simulations	33
4.1	Summary of $2\ \mu\text{m}^2$ AFM images of uncapped nanoparticles	35
6.1	Energy as a function of QDash height with and without WL	52
6.2	Three phosphorus concentration conditions	53
6.3	Three phosphorus concentration conditions bandgap diagram	54
6.4	Three phosphorus concentration conditions in the wetting layer	55
6.5	Phosphorus concentration conditions (2) and (3) in the wetting layer	55

6.6	Effect of QDash height on overlap integral	56
6.7	Effect of QDash width and length on overlap integral	57
6.8	Effect of sublayer thickness on overlap integral for GaAs and GaP.	58
6.9	Effect of phosphorus concentration on overlap integral for GaAs and GaP sub-	
	layers.	58
8.1	Overview of GaAs $1\ \mu\text{m}^2$ AFM images	62
8.2	Overview of GaP $1\ \mu\text{m}^2$ AFM images	63
8.3	Overview of height distribution plots for GaAs sublayer $1\ \mu\text{m}^2$ AFM images	64
8.4	Overview of height distribution plots for GaP sublayer $1\ \mu\text{m}^2$ AFM images	65
8.5	Reference guide for processing box.qdd information	83

Chapter 1: Introduction

Semiconductor mode-locked multiwavelength quantum dash (QDash) lasers are ideal for telecommunications applications due to their compactness, robustness, and low cost [4]. Multi-wavelength lasers have the ability to replace many separate lasers operating at single channels with a single chip, thus reducing cost and power consumption [5]. Quantum dot (QDot) and dash (QDash) gain media have advantages over their standard quantum well (QW) and bulk devices such as lower temperature dependence, better stability, and higher gain [4]. This is enabled by the increased discretization of the density of states that occurs as the dimensionality of the system is reduced.

Semiconductor QDots and QDashes for telecommunications applications are grown epitaxially. They can be grown with chemical beam epitaxy (CBE), metalorganic chemical vapor deposition (MOCVD), or molecular beam epitaxy (MBE). The QDashes and QDots analyzed using atomic force microscopy (AFM) in this thesis are grown using CBE. These nanoparticles grow via the self-assembled Stranski-Krastanow growth mode, spontaneous islanding that forms as a result of lattice mismatch between the substrate and epilayer. There are thus nuances and intricacies to their morphology and composition that are of interest in this thesis.

Earlier QDot lasers were developed with the InAs/GaAs material system, where the large lattice mismatch of approximately 7% induced well-defined QDots that emitted in the 1.3 μm regime when pumped. This corresponds to the O- and E-bands of optical telecommunications. For the long-haul telecommunication conventional band (C-band), operating at a centre wavelength of ~ 1550 nm, InAs/InP materials are more convenient. However, since the lattice mismatch between InAs and InP is approximately half that of the InAs/GaAs system, self-assembled nanoparticles can take the form of either QDots or QDashes depending on growth conditions [3], [6]. While QDots are zero-dimensional systems with equivalent lateral dimensions, QDashes are elongated in one lateral dimension. They are therefore considered quasi-one-dimensional systems that still confine carriers in all three dimensions like QDots, but have weaker confinement in the elongated direction. InAs/InGaAsP/InP QDash lasers are being grown and characterized at National Research Council (NRC) Canada. Using samples grown at NRC and accompanying photoluminescence data, this thesis characterizes InAs/InGaAsP/InP QDashes and develops a model to study the energy levels within a single QDash.

1.1 History and Background

The idea of two- and three-dimensional quantum confinement for increased laser performance was first published by Arakawa and Sakaki in 1982 [7]. Now known as quantum wire (QWire) and quantum dot lasers (QDotLs), respectively, this concept was introduced as the “multidimensional (2D or 3D) quantum well (MD-QW) laser” [7]. Preliminary theoretical studies of this device indicated promising beneficial effects including temperature insensitive threshold currents and improved laser device performance. For QDotLs, Arakawa and Sakaki predicted an effective temperature independence of the threshold current. This theory predated the successful procedure for semiconductor self-assembled quantum dots, a process which was first documented in 1985 by Goldstein et al., where molecular beam epitaxy produced three-dimensional “islands” of InAs on a GaAs substrate in arsenic-rich conditions [8], [9].

The discovery that semiconductor quantum dots would form under correct growth conditions buoyed researchers’ confidence in the realization of quantum dot fabrication processes. In 1994, two concurrent discoveries took place. The first is credited for initially garnering attention for the potential of quantum dot lasers, where Kirstaedter et al. used the Stranski-Krastanow growth method to create In(Ga)As quantum dots using self-assembly for low threshold lasing emission [10], [11]. That same year in Fujitsu Laboratories, Japan, atomic beam epitaxy was used by researchers Mukai et al. with the initial goal of creating InGaAs superlattices for high efficiency 1.3 μm emission. Instead, they also found that InGaAs would self-assemble on GaAs substrates due to the lattice mismatch between the two alloys, creating quantum dots that had emission wavelengths at 1.3 μm and were ideal for telecommunications applications [12], [13]. With this discovery came the knowledge that QDotLs could revolutionize the optical communications industry [13], [14].

QDotLs and quantum dash lasers (QDashLs) are now used in various applications including telecommunications and have been commercialized since 2011. Current telecom QDotLs offer superior performance for some metrics, including the reduction of threshold currents and their temperature sensitivities, reduced chirp, broader bandwidths that facilitate higher transport of data, and faster carrier dynamics [15]. These devices are pushing the boundaries of the telecoms industry for next generation optical networks and increased accessibility to data to remote communities [15].

1.2 Motivation and Structure

The construction of increasingly efficient QDashLs is a fast-moving field, where simulations of these devices and their constituents are invaluable for informing the growth of new designs. The effect of changing the structure and composition of single QDash on emission energy is integral in facilitating the growth of improved designs. This thesis discusses nanostructure heterojunction energy level calculations and links them to the properties of InAs nanoparticles grown on materials lattice-matched and strained to InP substrates. AFM measurements are performed on samples of InAs/InGaAsP/InP QDashes grown under various growth temperatures to understand the effect of growth parameters on island formation, and for dimensional analysis. Single InAs/InP QDash simulations are developed using Crosslight Photonic Integrated Circuit Simulator (PICS3D) software [16]. Results from AFM analysis are used to inform the simulated QDash dimensions. There is some overlap between results in the two publications included in this thesis, as the procedure for analyzing uncapped QDashes is established in one and utilized in the other.

This thesis introduces relevant theory in Chapter 2, needed to understand the research described in later chapters. A review of band theory, strain, density of states, and electron transition rules is presented, followed by the mechanisms by which nanoparticles spontaneously form during epitaxial growth.

Chapter 3 contains the experimental methods for AFM experiments, as well as a thorough outline of the developed procedure for analyzing the resulting AFM images. The next section is a description of the software Crosslight PICS3D, and explains the simulation setup process and relevant parameters included in the model. This section also includes a discussion about how to establish a finite element mesh for a dynamic structure.

Chapter 4 presents a conference proceeding for Photonics West 2022, published through the Proceedings of SPIE 12010 in March 2022. This publication describes the analysis of uncapped QDashes through AFM measurements, and draws a correlation between the height of the uncapped QDashes and the emission wavelength of their buried counterparts, measured through photoluminescence. The samples analyzed were grown and measured by photoluminescence at National Research Council Canada, and AFM experiments and analysis were done by the author at the University of Ottawa.

Chapter 5 of this thesis presents the manuscript of a journal article ready to be submitted to Applied Physics Letters about some of the results collected and analyzed from the single QDash

simulations. Results about the effect of QDash height, length, and width are discussed, as well as the effect of sublayer type and thickness, and phosphorus concentration of the QDash and associated wetting layer (WL) on the emission energy.

For completeness, Chapter 6 continues with single QDash simulation results, in particular the effect of WL structure and composition on energy levels and predicted emission wavelength. An analysis of the overlap integrals for simulation results is also discussed.

Chapter 7 summarizes the scope of the thesis, and provides recommendations for further experiments, simulations, and methods to continue with this work. Limitations of the model are discussed, with the goal of giving direction to future work. The Appendix of this thesis provides all the AFM images resulting from the AFM analysis for the reader to peruse at their leisure, and an example of a band theory that could be useful for future versions of this model. The raw code used to model the single QDash in Crosslight PICS3D is also provided.

Chapter 2: Theory and Background

2.1 Band Structure and Single Band Parabolic Model

In crystalline materials, the interaction of adjacent atoms and their electrons in a periodic lattice produces energy bands. The electrons per atom are arranged in orbitals; when a crystal lattice forms these orbitals overlap and hybridize. This hybridization is responsible for the presence of the energy gap in semiconductors: bonding orbitals form the valence band (VB), and antibonding orbitals form the conduction band (CB). At equilibrium and at 0 K, the highest energy level occupied by electrons is known as the valence band edge (with energy E_v at the band edge), and the lowest energy level that is left unoccupied is the conduction band edge (CB, with energy E_c at the band edge). The energy difference between these two bands is referred to as the bandgap of the bulk material, with energy $E_g = E_c - E_v$. This is shown in Fig. 2.1. This is a forbidden region where there are no energy levels for electrons to occupy, due to the energy splitting between bonding and antibonding orbitals. If electrons in the VB are excited with an energy $E \geq E_g$, they can overcome the energy gap and enter the CB, leaving behind a hole. Holes are positively charged massive quasi-particles that act as the charge carriers in semiconductors along with electrons. The magnitude of the bandgap is determined by the composition of the semiconductor and is largely dependent on the strength of atomic bonds that dictates the level of splitting between orbitals. In general, for larger elements further down the periodic table, the bonds are weaker due to reduced electronegativities and splitting is less, therefore producing semiconductors with smaller bandgaps.

We can consider our energies as a function of $\mathbf{k}$, the reciprocal lattice wavevector. In the parabolic band approximation, the dispersion relation for either holes or electrons (VB or CB) is given by the following equations:

$$E_v(\mathbf{k}) = E_v - \frac{\hbar^2 k^2}{2m_0 m_h} \quad (1)$$

$$E_c(\mathbf{k}) = E_c + \frac{\hbar^2 k^2}{2m_0 m_e} \quad (2)$$

In the above equations, m_h , m_e refer to the effective mass of either holes or electrons, $\hbar$ is Planck's constant, and m_0 is the mass of a free electron. In the more detailed case below where there is valence band splitting, we obtain two separate bands for heavy and light holes with effective masses $m_h = m_{HH}$ or m_{LH} , respectively. These result from the energy required for a

charge carrier to travel in different crystal planes, represented as varying effective masses. This simple model of the bandgaps of semiconductors is referred to as the **parabolic model** and will be the basis for the simulations discussed in this thesis. It is a very simple approximation of the band structure of semiconductors, where the $k = 0$ point captures the band edges for direct bandgap materials and is referred to as the Γ point.

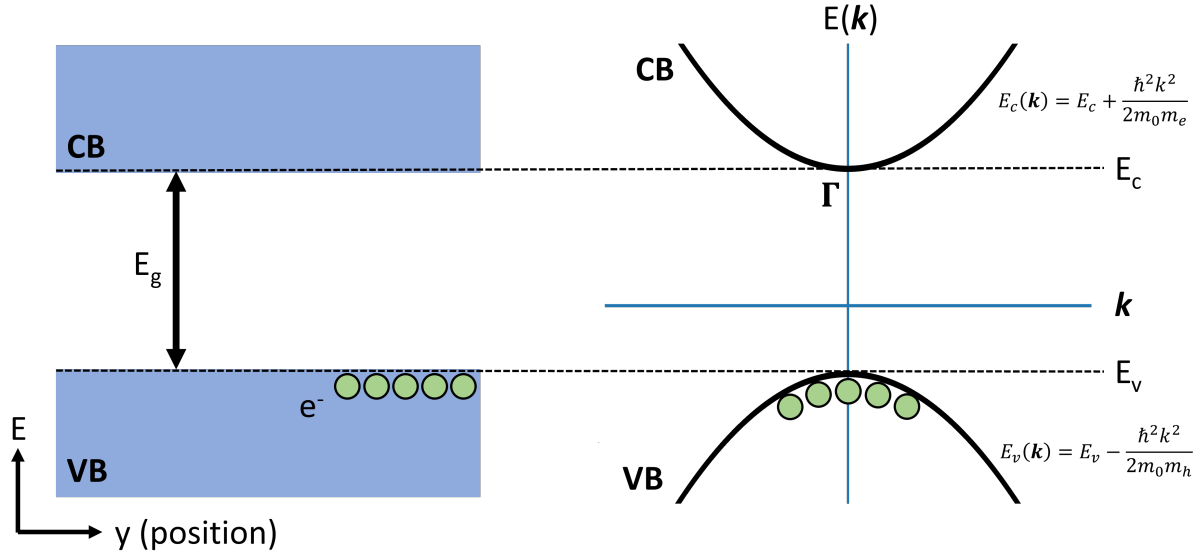


Figure 2.1: General simplified bandgap diagrams in real (left) and momentum (right) space.

2.1.1 Zinc-Blende Semiconductors

For the binary (InAs, GaAs, GaP, InP), ternary (InAsP), and quaternary compounds (InGaAsP) considered in this thesis, the hybridized sp^3 orbitals are what induces the tetrahedral shape characteristic of zincblende crystals. Due to their electronic structure, with eight valence electrons per two atoms, they are referred to as p-block octet semiconductors. The binaries included in the scope of this thesis are presented in Fig. 2.2. All of these compounds form direct band gaps at the Γ ($k = 0$) point, which means that the lowest point of the CB and the highest point of the VB are aligned: a hole and an electron at these points will have the same k value. Thus an electron transition from the CB to the VB at this point does not need a change in momentum to occur, and will readily emit a photon. In contrast, electrons in materials with indirect band gaps - where the maxima and minima of the VB and CB are not aligned in k - will require a change in momentum for a transition and photon emission to take place.

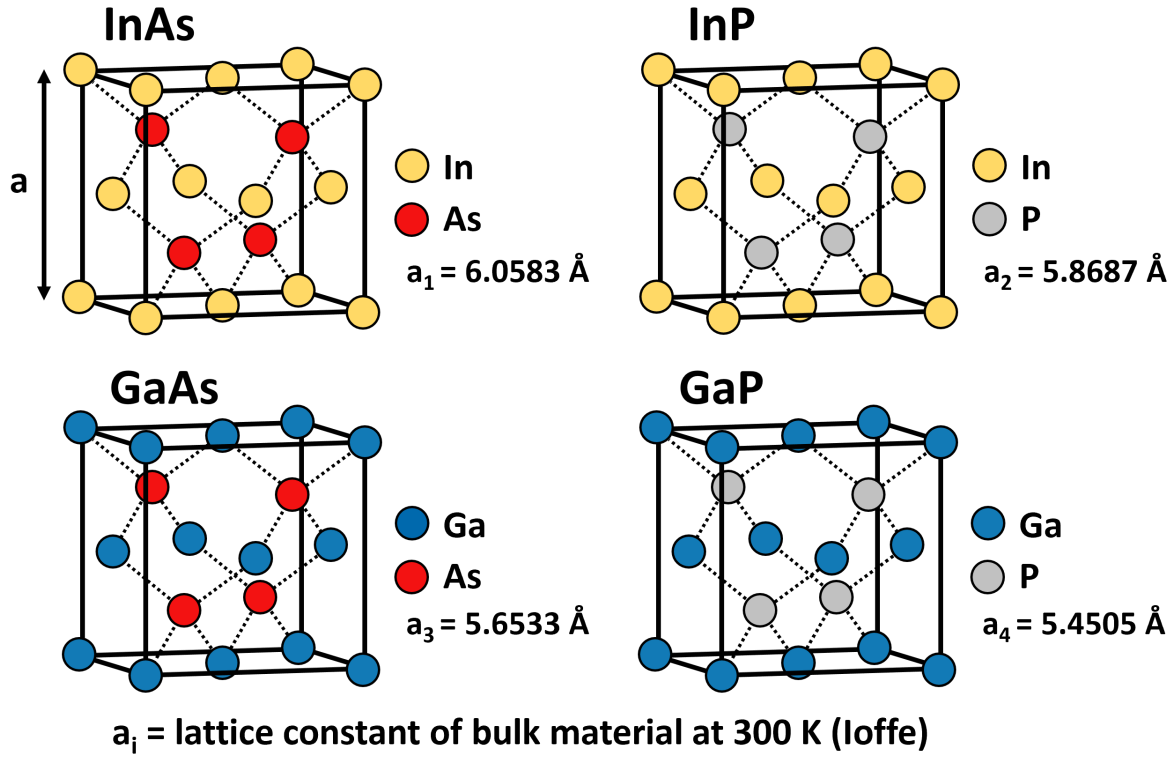


Figure 2.2: Zincblende cubic unit cells and lattice constants for the III-IV binary compounds relevant for this thesis.

2.1.2 Valence Band Splitting and Strain

The symmetry of the hybridized orbitals leads to splitting of the VB into two bands. Consider an electron in a zincblende crystal lattice. Depending on the crystallographic direction of electron propagation, the overlap of adjacent atomic orbitals varies. This variation is one of the driving factors in the effective mass difference between the two highest energy valence bands. The tops of the valence bands have p -symmetry, meaning that their shape in momentum space is largely determined by the p_x , p_y , and p_z orbitals. Similar semiconducting crystals form in alloys of group IV atoms, or by mixing group I, II, or III with VII, VI, or V respectively.

There are two different valence bands: the heavy hole (HH) band, with larger effective mass, and the light hole (LH) band, with lower effective mass. If we consider our equation Fig. [1](#), we can see that the lighter and heavier hole masses represent bands of different curvature in Fig. [2.4](#). There is also a third band known as the split-off (SO) band that occurs due to spin-orbit coupling. This split-off band is usually separated from the LH and HH bands by many hundreds

of meV in III-V compound semiconductors due to their comparatively high atomic number, and is therefore not considered further in the scope of this thesis. The single band parabolic model used in these simulations approximates the HH and LH bands by assuming no coupling between the two of them. This is an acceptable simplification for low energy approximations, however it should be noted that the energy difference between the bands is small enough that valence band states are rarely purely light or heavy; there is coupling between the bands. A possible extension to these simulations which is discussed in section [8.4.1](#) that includes these effects is the $\mathbf{k} \cdot \mathbf{p}$ method. This is a perturbation theory that expands around a specific k -value to solve for the band structure around the band edges.

The LH and HH band formation is a result of the different effective masses of the electron depending on the direction of its motion. In the bulk unstrained case, the HH and LH bands are degenerate at the Γ point. However, disruption of the crystal symmetry, for example via strain or quantum confinement, removes this degeneracy and introduces valence band splitting. Strain modifies the positioning of orbitals in the lattice and their energies. Thus, both quantum confinement and strain work together in this respect to modify the VBs and remove the degeneracy that is characteristic of bulk unstrained systems.

The strain can be induced by a mechanical force applied to the lattice, or in the case of epitaxial growth, by the difference in lattice constant between subsequently grown semiconductors. At the interface of two semiconductors, for thin epilayers, the deposited semiconductor will deform to match the lattice constant of the substrate, therefore inducing strain in the epilayer. If the lattice constant is larger (smaller) than the substrate, the resulting epilayer is under compressive (tensile) strain. For thin layers under the critical layer thickness, this strain will be maintained in the layer and the entire lattice will elastically deform to lattice-match the substrate. Beyond the critical layer thickness, dislocations are energetically favourable at the interface to relieve strain and allow the epilayer to return to its unstrained lattice constant. As evident in Fig. [2.3](#), distortion in the crystal lattice will introduce anisotropy in the valence bands, shown in Fig. [2.4](#).

For compressive strain, where the lattice constant of the epilayer decreases in the x, y plane, the energy of the p_z orbital decreases and thus the top valence band follows the shape of p_x and p_y orbitals. This is shown in Fig. [2.4\(b\)](#), where solid VBs correspond to compressively strained systems, and dashed VBs to tensile strained systems. These orbitals facilitate faster electron transport in the x, y lattice plane and are thus "light" in $k_{x,y}$; the curvature of the top band for compressively strained semiconductors is anisotropic: higher curvature in the $k_{x,y}$ direction and shallower in the k_z direction. The lower band in this case follows the opposite rule. For tensile strained systems, the opposite is true: the top VB is "light" i.e. more curved in the k_z direction

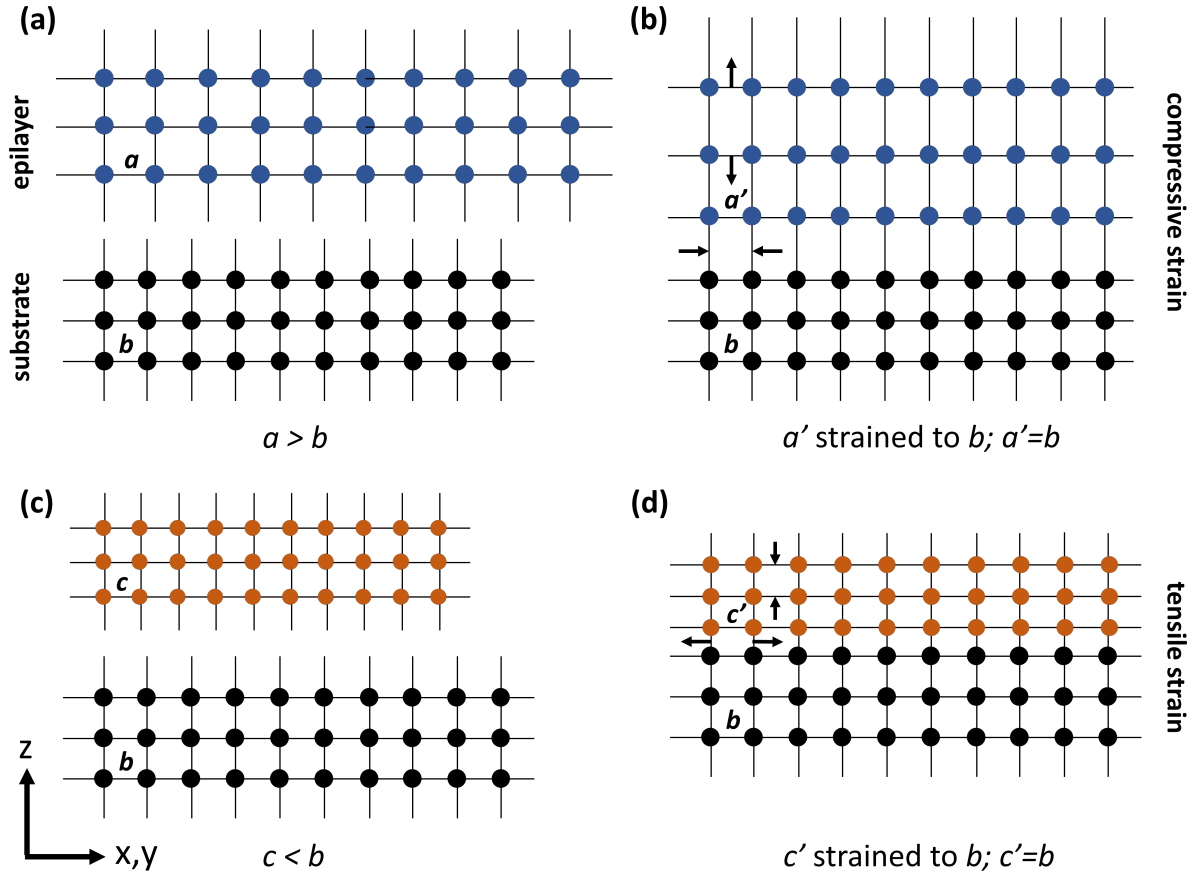


Figure 2.3: (a) Substrate with lattice constant b , and second material with lattice constant $a > b$; (b) Deposition of material epilayer onto substrate where lattice constant of epilayer compresses to match substrate (compressive strain); (c) Material with lattice constant $c < b$; (d) Deposition of material epilayer onto substrate where lattice constant of epilayer expands to match substrate.

due to a compression of the epilayer in z , and "heavy" i.e. less curved in the $k_{x,y}$ direction. Again, the lower band portrays the opposite behaviour to the upper band.

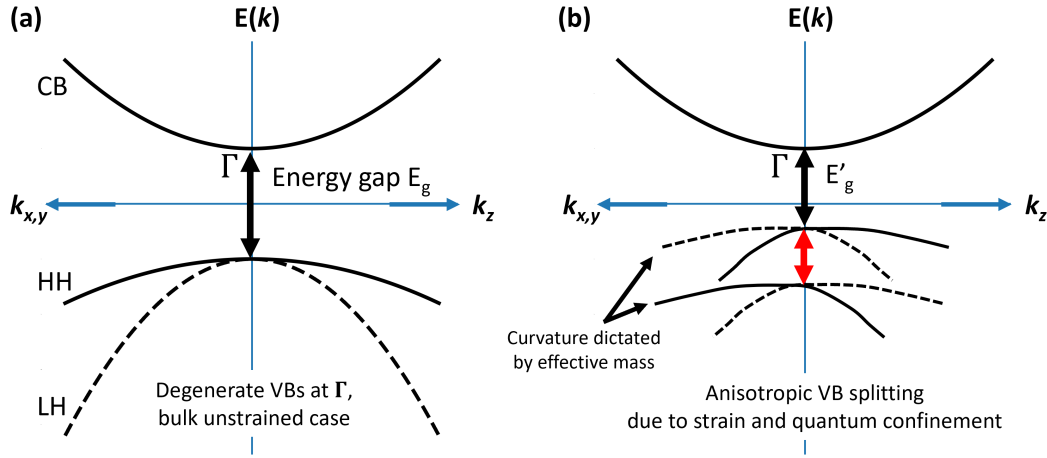


Figure 2.4: (a) General bandgap diagram for bulk unstrained system in terms of wavevector k , with conduction band (CB), heavy hole (HH), and light hole (LH) bands for direct bandgap semiconductor at the Γ point; (b) Bandgap diagram depicting splitting of LH and HH bands at the Γ point due to strain/quantum confinement in the semiconductor. Modified from [17].

2.1.3 Quantum Confinement

In a simple double-heterojunction structure, where a lower bandgap material is sandwiched between a higher bandgap material, the charge carriers are confined in one dimension to the lowest bandgap region of the structure [18]. If this low bandgap region thickness is on the order of the de Broglie wavelength of the charge carriers λ_{DB} , the system behaves as a finite potential well in which the carriers experience quantum confinement.

Confining an electron in a QW causes discretization of the electron's energy levels in one dimension. When this concept of carrier confinement is extrapolated to two and three dimensions, the systems are known as QWires, QDashes, and QDots. Quantum wells, wires, dashes, and dots can be referred to as two-dimensional, one-dimensional, quasi-one-dimensional, and zero-dimensional structures, respectively. The electron's energy levels within a QDot are analogous to the discrete energy levels described by the Bohr-Rutherford model [19].

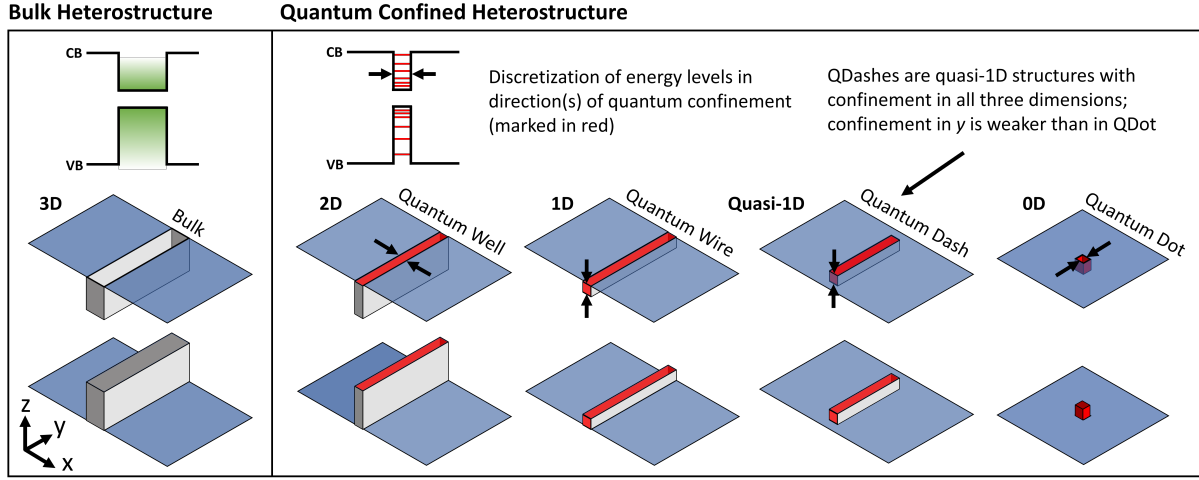


Figure 2.5: Confining heterostructure with example energy levels shown for bulk layers (left) and quantum structures (right).

2.1.4 Band Alignment

The alignment of bandgaps of specifically chosen semiconductor materials are used to energetically prohibit transport of charge carriers by creating wells or barriers in what is known as bandgap engineering. There are three main forms of band alignments in heterostructures, classified by the VB and CB offsets between adjacent semiconductors and shown in Fig. 2.6: (a) type I straddling alignment, where both electrons in the CB and holes in the VB are confined; (b) type II staggered alignment, where electrons and holes are either confined or blocked by a potential well or barrier; and (c) type III broken gap alignment, where the bandgaps of adjacent materials do not overlap at all and charge transfer between the VB and CB of each material occurs spontaneously until the induced electronic field prevents this process [17]. An increasing magnitude of the band offset - the energy difference between the edge of the adjacent bands - increases confinement and affects the allowed energy levels of carriers within the confining region, to be discussed in further detail in Chapter 5.2 of this thesis.

Anderson's rule is used to determine the alignment of the bandgaps, and is based on vacuum levels and electron affinity. The electron affinity is defined as the energy required to excite an electron from the conduction band edge to vacuum level, where it has enough energy to leave the crystal [17]. Anderson's rule states that the vacuum levels of adjacent materials in a heterostructure must line up. This determines the conduction band offset (CBO), the change in conduction band level between adjacent materials. The valence band offset (VBO) is then established based on the difference in bandgaps between the materials.

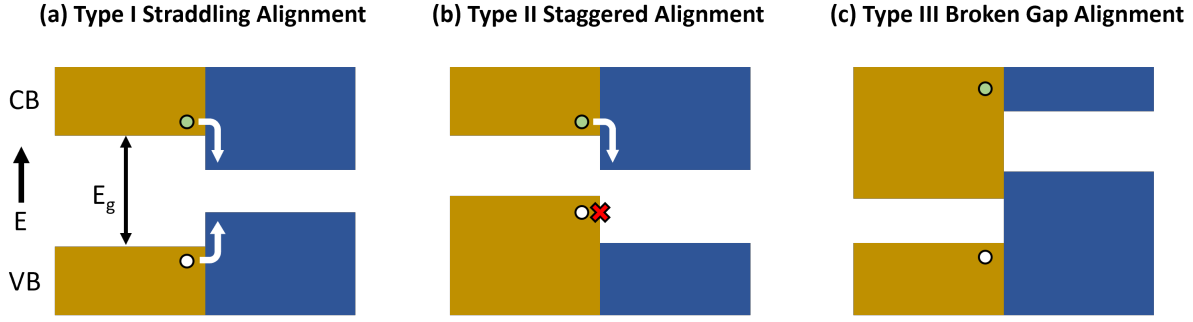


Figure 2.6: Three Band Alignments for Heterostructures (a) Type I Straddling Alignment; (b) Type II Staggered Alignment; (c) Type III Broken Gap Alignment.

2.2 Density of States

The density of states of a material defines the number of available states per unit volume at a specific energy. In bulk materials, the density of states as a function of energy is continuous and parabolic [19], [20]. This means that for increasing energy there are an increasing number of states available for electrons to occupy. The total carrier density (density of occupied states) is given by the product of the density of states function $\mathcal{D}(E)$ and the probability of occupation $f(E)$, integrated over all energies:

$$n = \int_{-\infty}^{\infty} \mathcal{D}(E) f(E) dE \quad (3)$$

The probability of state occupation is given by the Fermi-Dirac distribution:

$$f(E) = \frac{1}{\exp\left(\frac{E - E_F(T)}{k_B T}\right) + 1} \quad (4)$$

For a bulk material, the resulting carrier density is distributed continuously over a range of energies. As the dimension of confinement increases, quantization effects begins to discretize the density of states. For quantum wells, a step-like density of states forms, and for quantum wires and quantum dashes, the density of states is as shown in Fig. 2.7.

For ideal QDots, carrier confinement in all three dimensions within such a small volume leads to the full discretization of the density of states, as shown in Fig. 2.7, and therefore the number of states available per unit volume is confined to a small spread of allowed energy values and follows a Dirac delta distribution. Consequently, a change in the Fermi function or change in temperature of the system has minimal effect on the carrier distribution [19]. The narrowing of the density of states in QDots and QDashes is therefore what makes them so promising for laser

gain media, as this phenomenon directly reduces the threshold and injection currents, weakens the temperature dependencies, and reduces the number of injected carriers required to satisfy the condition of population inversion [19], [21].

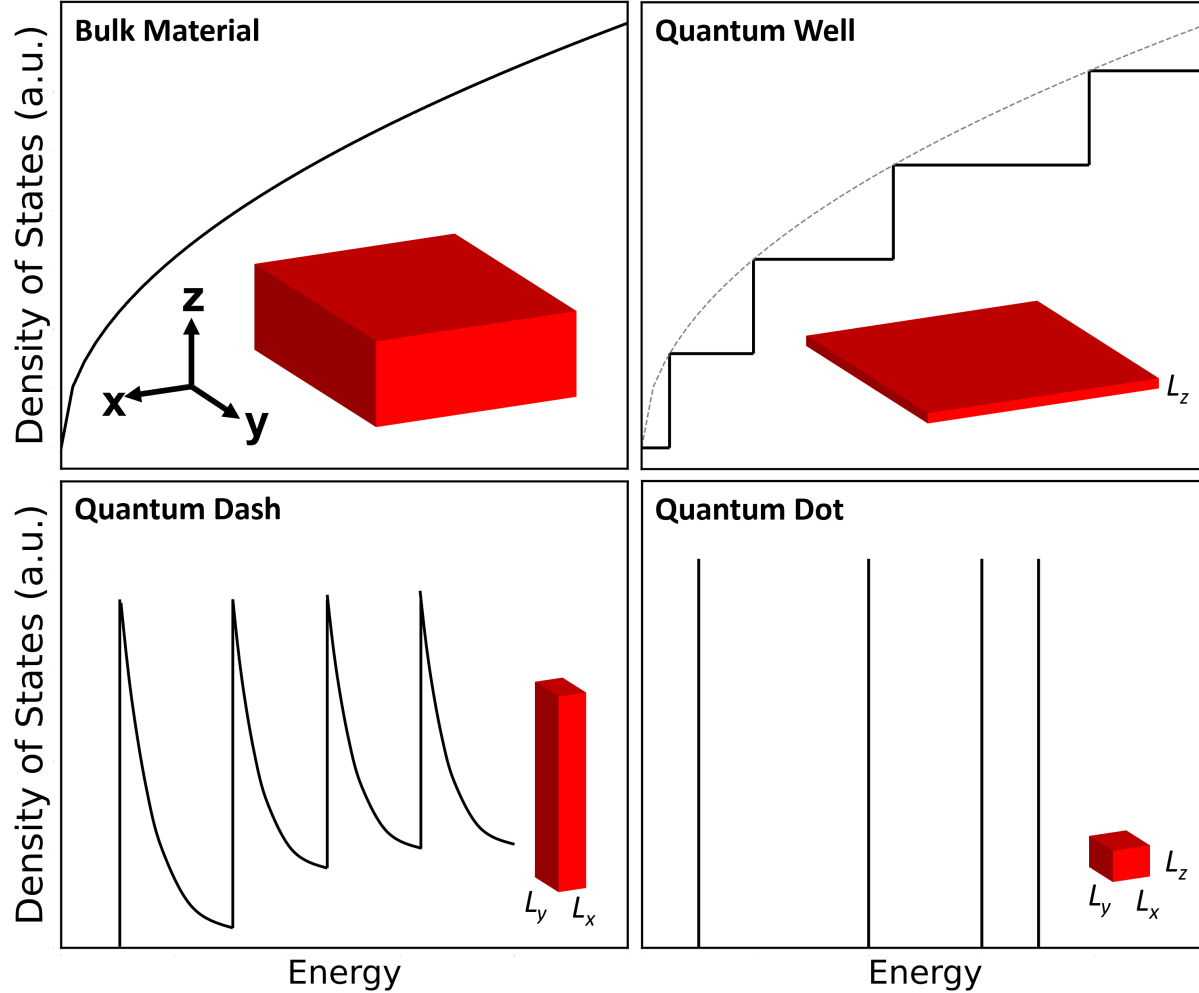


Figure 2.7: Summary of idealized density of states as a function of energy (a.u. for both axes).

2.2.1 Ideal Density of States Derivations

Free Electron - 3D

More details about these derivations can be found in [17], [22]. To begin deriving the density of states for various levels of electron confinement, we can start with the three-dimensional time-independent Schrödinger equation:

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + \mathbb{V}(\vec{R}) \right) \Psi_{\vec{k}}(\vec{R}) = E \Psi_{\vec{k}}(\vec{R}) \quad (5)$$

Where we define $\vec{R} = (x, y, z)$ and $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$. $\mathbb{V}(\vec{R})$ represents the potential, Ψ is the wavefunction of the particles, $\vec{k}$ is the wavevector, and E is the energy of the particle. With free electrons, the potential is zero and the particles would travel freely in a volume V as plane waves of the following form and with energies $\epsilon_{\vec{k}}$ and ϵ_F given by:

$$\Psi(\vec{R}) = \frac{1}{V} \exp(i\vec{k} \cdot \vec{R}); \epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}; \epsilon_F = \frac{\hbar^2 k_F^2}{2m} \quad (6)$$

With the density of points is represented as $\frac{V}{(2\pi)^3}$ in reciprocal space (k -space), the number of states within a spherical volume can be written as the product of the density of points and the volume integral using the surface area of a sphere up to the Fermi wavevector (multiplied by a spin degeneracy factor of two to account for spin):

$$N = 2 \left(\frac{V}{8\pi^3} \right) \int_0^{k_F} 4\pi k^2 dk = \frac{V k_F^3}{3\pi^2} \quad (7)$$

The electron density n is the above divided by the volume, N/V , and we can substitute this into the above equations to get the electron density as a function of energy:

$$n(\epsilon) = \frac{1}{3\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{3/2} \quad (8)$$

Finally, the density of states is given by the derivative of the electron density with respect to energy. This gives us the general expression for the density of states for a three-dimensional volume of free electrons:

$$\mathcal{D}(\epsilon) = \frac{\partial n(\epsilon)}{\partial \epsilon} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} \quad (9)$$

Quantum Well - 2D

If we now lower the dimensionality of the system to two, and confine particles in the z -direction, we can express this as a potential $V(z)$ in our Schrödinger equation:

$$\left(\frac{-\hbar^2}{2m} \nabla^2 + V(z) \right) \Psi_{n,\vec{k}}(\vec{R}) = E \Psi_{n,\vec{k}}(\vec{R}) \quad (10)$$

Where n is the subband number. If we assume a lateral plane wave as an appropriate solution based on symmetry, a possible solution is thus of the form:

$$\Psi_{n,\vec{k}}(x, y, z) = \exp(ik_x x) \exp(ik_y y) \phi_n(z) \quad (11)$$

with $\left(\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial z^2}\right) + V(z)\right)\phi(z) = \epsilon_n\phi(z)$. The total energy as a function of the subband energy ϵ_n and wavevector $\vec{k}$ is given by:

$$\epsilon_{n,\vec{k}} = \epsilon_n + \frac{\hbar^2 \vec{k}^2}{2m} \quad (12)$$

Following the same process as in our three-dimensional case, we can find our expression for the total number of states in the system, calculate the electron density, and then take the derivative with respect to energy to get the density of states for a two-dimensional structure (such as a quantum well). Note that for our total number of states, an integral is used for our two unconfined dimensions (continuous), and a summation is used for the confined dimension (discretized):

$$N_{2D} = 2 \sum_{n \text{ filled}} \frac{L^2}{(2\pi)^2} \int_0^{k_F} 2\pi k dk = \sum_{n \text{ filled}} \frac{L^2 k_F^2}{2\pi} \quad (13)$$

$$n = \frac{N_{2D}}{L^2} = \sum_{n \text{ filled}} \frac{k_F^2}{2\pi} = \sum_{n \text{ filled}} \frac{m}{\pi\hbar^2} (\epsilon - \epsilon_n) \quad (14)$$

$$\mathcal{D}(\epsilon) = \frac{dn}{d\epsilon} = \frac{m}{\pi\hbar^2} \sum_{n \text{ filled}} \Theta(\epsilon - \epsilon_n) \quad (15)$$

In the above expression for the density of states, $\Theta(\epsilon - \epsilon_n)$ is the Heaviside function.

Quantum Dash and Quantum Wire - 1D

Let's increase the degree of confinement once more. For a system with two-dimensions of quantum confinement, x and y , we follow the same process as above with a potential of the form $V(x,y)$ and adding an additional subband term for the discretized axis:

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(x,y)\right)\psi_{m,n}(x,y) = E\psi_{m,n}(x,y) \quad (16)$$

Where m and n are subband quantum numbers in each dimension of confinement. Similarly, our energies and wavefunctions take the following form:

$$\left(\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y)\right)\psi_{m,n}(x,y) = \epsilon_{m,n}\psi_{m,n}(x,y) \quad (17)$$

The density of states for this system is given by:

$$\mathcal{D}(\epsilon) = \frac{(2m)^{1/2}}{\pi\hbar} \sum_{m,n \text{ filled}} (\epsilon - \epsilon_{m,n})^{-1/2} \Theta(\epsilon - \epsilon_{m,n}) \quad (18)$$

Quantum Dot - 0D

The density of states for an ideal QDot assumes full discretization in each dimension. It can be written as the following, where l , m , and n are the quantum subband numbers for each dimension of confinement, x , y , and z .

$$\mathcal{D}(\varepsilon) = 2 \sum_{l,m,n \text{ filled}} \delta(\varepsilon - \varepsilon_{l,m,n}) \quad (19)$$

2.3 Electron Transition Rules

The simulations presented in this thesis are established to approximate the energy levels within single QDash structures. When we discuss the concept of transition wavelength and energy, we are considering the energy an electron must release to drop from the first subband of the conduction band Γ valley to the first subband of the heavy hole valence band.

2.3.1 Scattering Processes

Fig. [2.8](#) describes the three main interband light scattering processes that occur in a defect-free semiconductor: (1) absorption, (2) spontaneous emission, and (3) stimulated emission. In (1), an incident photon with energy $E = E_g$ is absorbed by an electron in the VB. The electron is excited to the CB. For semiconductor lasers, this process is known as pumping the gain medium. In (2), electrons in the excited state can relax and release energy. In this process, a photon with an energy equal to the gap between energy levels the electron travelled is released. Photons generated in the gain medium through spontaneous emission can then induce (3) stimulated emission, the process by which the laser earned its name. Stimulated emission is the induced release of energy from an excited electron by incident light.

If an incoming spontaneous photon possesses the energy similar to the energy of a specific transition, it can induce the transition and stimulate the emission of a photon coherent and in-phase with the incoming photon. If population inversion is fulfilled, where there must be more electrons in the excited state than the lower state, light amplification via stimulated emission will occur and the lasing condition is satisfied. In QDash lasers, the discretized energy levels in the QDashes dictate the emission wavelength of each individual photon generated in each QDash in an array within the gain medium. It is therefore crucial to understand how the structure and composition of the individual QDashes affect the bandgap structure and energy levels in the nanoparticle since this will directly affect the laser properties.

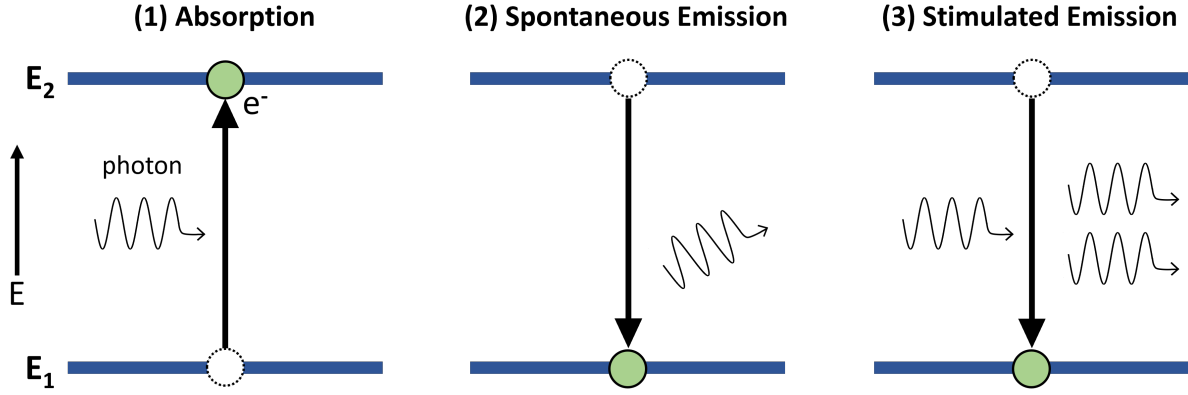


Figure 2.8: (1) Absorption process where incident photon excites electron to higher energy level; (2) Spontaneous emission where electron relaxation emits photon; (3) Stimulated emission where incident photon induces relaxation of electron and emission of photon coherent with itself.

2.3.2 Fermi's Golden Rule

The equations contained in this section are based on [17]. Fermi's Golden Rule for optical absorption is shown below. It gives an expression for the transition rate of an electron from a state i in the valence band to state f in the conduction band due to the absorption of a photon.

$$W_{fi} = \frac{2\pi}{\hbar} \left(\frac{eE_0}{m_0\omega} \right)^2 |\langle f | \mathbf{e} \cdot \hat{\mathbf{p}} | i \rangle|^2 \delta(E_f - E_i - \hbar\omega) \quad (20)$$

In the above equation, $\hbar$ is Planck's constant, E_0 is the electric field (constant), m_0 is the free electron mass, ω is the frequency, and f and i refer to the final and initial states, respectively. E_f and E_i therefore refer to the energy of the final and initial states. The electric field E_0 is treated as constant since the wavelength of incident photon is much larger than the extent of the electronic wave function. The term in front of the matrix element is thus considered constant. The optical matrix element contains $\mathbf{e} \cdot \hat{\mathbf{p}}$, the dot product of the light polarization vector and the momentum operator. The delta function stipulates that transition will only occur if the difference between the energies of the final electron state E_f , initial electron state E_i , and energy of the photon $\hbar\omega$ is zero. Taking a closer look at the optical matrix element, we have:

$$\mathbf{e} \cdot \hat{\mathbf{p}} = -i\hbar \left(e_x \frac{\partial}{\partial x} + e_y \frac{\partial}{\partial y} + e_z \frac{\partial}{\partial z} \right) \quad (21)$$

The total power absorbed in the system must take into account that the final state must be empty and the initial state is filled. It does this by utilizing the Fermi function described earlier in

equation 4. The total rate of absorption of energy is also summed over all possible final and initial states:

$$P = \frac{2\pi}{\hbar} \hbar\omega \left(\frac{eE_0}{m_0\omega} \right)^2 2 \sum_{i,f} |\langle f | \mathbf{e} \cdot \hat{\mathbf{p}} | i \rangle|^2 (f(E_i) - f(E_f)) \delta(E_f - E_i - \hbar\omega) \quad (22)$$

How can we tell if a transition will occur and which transition is most probable? This is dictated through selection rules, and can also be approximated numerically. Let's look at transitions in the simplest case of a low-dimensional system, the quantum well. For a transition between the VB and CB in a quantum well, the optical matrix element can be simplified to the following, where cn is a bound final state n in the conduction band with $\mathbf{k} = \mathbf{k}'$ and vm is a bound initial state m in the valence band with $\mathbf{k} = \mathbf{k}$:

$$\langle f | \mathbf{e} \cdot \hat{\mathbf{p}} | i \rangle \approx \langle cn\mathbf{k}' | \mathbf{e} \cdot \hat{\mathbf{p}} | vm\mathbf{k} \rangle \quad (23)$$

Envelope functions in a quantum well have the simplified form of a plane wave in x , y , and a bound state in z (assuming quantization in z). These envelope functions take the form $\chi_c(\mathbf{r}) = A^{-1/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \phi_{cn}(z)$ or $\chi_v(\mathbf{r}) = A^{-1/2} \exp(i\mathbf{k} \cdot \mathbf{r}) \phi_{vm}(z)$, with the bound states represented by ϕ . The quantum well establishes that in order for a transition to occur, it must be vertical; $\mathbf{k}$ must be invariant. This simplifies equation 23 to:

$$\langle cn\mathbf{k}' | \mathbf{e} \cdot \hat{\mathbf{p}} | vm\mathbf{k} \rangle \approx \mathbf{e} \cdot \hat{\mathbf{p}}_{cn,vm} \delta_{\mathbf{k},\mathbf{k}'} \int \phi_{cn}^*(z) \phi_{vm}(z) dz \equiv \mathbf{e} \cdot \hat{\mathbf{p}}_{cn,vm} \delta_{\mathbf{k},\mathbf{k}'} \langle cn | vm \rangle \quad (24)$$

The above ensures that $\mathbf{k} = \mathbf{k}'$ for the final and initial states. There are two other selection rules that must be satisfied in order for a transition to occur.

(1) The overlap integral $\langle cn | vm \rangle$ dictates the quantum numbers m and n in the VB and CB, respectively, for an allowed transition and is independent of polarization and momentum. It is this selection rule that is most pertinent for the scope of this thesis. In the simplified infinite potential well, the overlap integral dictates that the transitions for $n = m$ are allowed. This is a decent approximation for a symmetric finite well, however asymmetric potentials can lead to transitions for $n \neq m$. In any case, this selection rule holds for asymmetric finite wells in that $n = m$ will give the strongest transitions. This overlap integral is calculated numerically in Crosslight. Crosslight will provide the overlap integrals as values from 0-1 for each set of quantum numbers (or subband indices). By default, the overlap integrals for transitions between the first ten quantum numbers in the HH and LH bands, and the Γ valley, are given. These overlap integrals can be used as an indicator of the most probable transition. In general,

the lowest energy transitions are for the HH- Γ bands, since the HH splits above the LH in the VB. The first sub-band of the heavy hole and Γ band transition, the HH1- Γ 1 transition, has the highest overlap integral in this dataset, and thus it is this transition that is taken as the predicted emission energy throughout this thesis.

(2) The optical matrix element gives rise to the polarization-dependent selection rule. The impact of this selection rule is beyond the scope of this thesis, however it must be noted that the polarization and propagation direction of light with respect to the low-dimensional structure will determine whether or not absorption is possible for LHs or HHs.

2.4 Self-Assembly of InAs/InP Nanoparticles

The spontaneous self-assembly of QDots and QDashes arises from the lattice mismatch and resulting strain between neighbouring semiconductor materials. InAs has a lattice parameter which is approximately 3.1-3.2% larger than that of InP, and thus InAs nanoparticles will self-assemble on InP substrates [18], [23], [24]. When growing thin film heterolayers, three types of growth processes may occur and are categorized by the interaction of the different layer materials. They are described in Fig. 2.9

Frank-van der Merwe growth refers to the two-dimensional epitaxial growth for lattice matched systems, or very slightly strained systems. This growth type occurs between two lattice-matched materials when the interaction between the substrate and the epilayer atoms is greater than the interaction between adjacent atoms of the film layer [25], in other words when the binding energy of the epilayer with the substrate is larger than the binding energy of the epilayer to itself [18]. Under these conditions, the epilayer is said to “wet” the underlying material to create a uniform wetting layer. The resulting structure is a thin film of uniform layers with no island formation, and the process is appropriately labelled layer-by-layer growth [19].

On the other extreme, Volmer-Weber growth occurs when layering highly lattice mismatched materials. In this growth process, small islands of one material form on top of another, with no intermediate uniform layer [18], [19]. This growth process occurs when the interaction between film atoms is greater than the interaction between the film and substrate atoms, since the binding energies between epilayer particles is larger than the binding energy between the epilayer and substrate [25]. Bonding between the epilayer and substrate would be energetically unfavourable, as the high lattice mismatch induces large strain between the two materials. By instead preferentially forming islands, the overall strain energy of the system is reduced [18],

[19].

The Stranski-Krastanow growth process is characterized by the initial growth of one or more monolayers of uniform thickness (a wetting layer) before islanding [25]. Again, this growth process occurs when the binding energy of the epilayer to the substrate is larger than the epilayer to itself, but with the added stipulation that the strain induced is non-negligible – that is, the semiconductor materials are not lattice-matched [18]. Self-assembled island formation occurs due to strain relaxation; in other words, the nanoparticles form to relax the overall energy of the system caused due to the lattice mismatch and strain. Stranski-Krastanow is the dominating growth process used for self-assembled QDots and QDashes, and is the process for common III-V nanoparticle materials such as InAs/GaAs and InAs/InP.

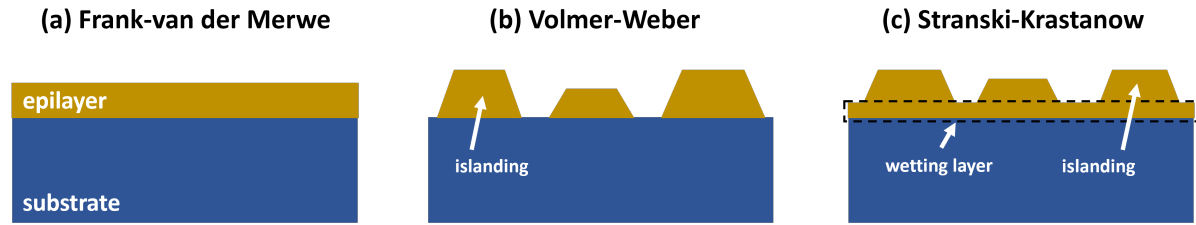


Figure 2.9: (a) Frank-van der Merwe growth; (b) Volmer-Weber growth; (c) Stranski-Krastanow growth.

The first self-assembled quantum dot (SAQD) lasers were created in 1994 using InAs on GaAs [10]. These devices emit in the 1.0-1.3 μm wavelength range and cannot easily be fabricated to emit in the C-band wavelength range (centred around 1550 nm). InAs/InP QDots/QDashes are attractive for exactly this application – InP-based self-assembled systems can emit at around 1.55 μm more easily [23]. The difference in emission wavelength between these two structures is due to the exchange processes and degree of strain between the respective materials. InAs has a 6.7% larger lattice constant than GaAs, and only a 3.1% difference compared to InP. A larger lattice mismatch allows InAs to more readily form nanoparticles on GaAs. In InAs/GaAs systems, the group III elements (In and Ga) are exchanged between the barrier and nanoparticle material, while in InAs/InP systems, the group V (As and P) materials are exchanged [23].

SAQDs can be grown by both molecular beam epitaxy and chemical beam epitaxy (CBE). The nanoparticles discussed in this thesis are grown by CBE. CBE forms epitaxial layers on a substrate through molecular gas beam deposition in an ultrahigh vacuum. More details about this process can be found in Chapter 3.1.1.

The following outlines the general process by which self-assembled InAs/InP QDots and

QDashes are grown on via CBE by Philip Poole at the National Research Council (NRC) [23], [26], [27]. More details can be found in reference [23], as this section was loosely based on the contents of this chapter. InAs nanoparticles can be grown either directly on a (001) oriented n-type InP substrate or on InGaAsP barriers, the latter of which is considered in this thesis. Thin GaP or GaAs sublayers on the InGaAsP barriers prior to InAs deposition can also be used to control the preferential formation of dots or dashes by modifying the strain, although they are not necessary for nanoparticle formation. GaP sublayers also promote higher dot density and layer uniformity when stacking layers of nanoparticles [28].

To begin the process of growing InAs dots, a thin layer of InAs highly strained to InP is deposited. Growth interruption then follows this deposition, allowing for Stranski-Krastanow growth to take place. The duration of growth interruption significantly impacts the final structure of the quantum nanoparticles. At short interruption times, the InAs layer shows distinct photoluminescence peaks as the layer begins to change thicknesses in step-like stages. As the interruption time increases, the resulting PL spectra becomes one smooth peak and QDashes form as islanding begins. Given sufficient time, QDots will form as the QDashes break up into smaller nanoparticles [23]. As growth interruption time increases, so too does nanoparticle height. The resulting structure after growth interruption is InAs QDots or QDashes present on an extremely thin InAs wetting layer.

Dashes form elongated in the $[0\ 1\ -1]$ direction, and have recorded heights from 5-15 nm (uncapped) or 2-3 nm (capped with InP); widths from 20-25 nm, and lengths ranging from 40 to hundreds of nanometres [3], [6], [23], [29]. QDots have similar heights but tend to be slightly taller, and average diameters from 25-40 nm.

These growths are usually performed at temperatures from 500-540°C. Growth temperature and As overpressure are crucial for controlling the growth of the nanoparticles, as higher temperatures and As overpressure will promote QDot over QDash formation [23].

After nanoparticles are formed, they are capped with InP. The capping procedure controls the final buried morphology of the QDots and QDashes, and can therefore be used to control the height and thereby emission energy. When capping with InP, the P flux incident on the particles induces In formation that in turn causes InP to creep from the top of the particles to the area between. This process is governed by the As/P exchange process, the effects of which are investigated in more detail in Chapter 6 of this thesis. Again, the duration of the capping process directly impacts the height of buried nanoparticles: longer capping procedures result in more As/P exchange, thereby flattening the top of the particles and further reducing their height. A double-capping procedure can also be utilized where a primary deposition of InP is followed

by a growth interruption that enables the As/P exchange before continuing with InP deposition. By splitting this procedure into two steps, taller particles are etched back preferentially to the already buried shorter ones, reducing the height distribution of the overall sample [23].

Chapter 3: Experimental Methods

3.1 Nanoparticle Growth

3.1.1 Chemical Beam Epitaxy

The nanoparticles analyzed in this thesis were grown using chemical beam epitaxy (CBE). The term epitaxy is derived from the Greek root words epi ("above") + taxis ("an ordered manner"). True to its name, epitaxy is a form of crystal growth where crystalline layers are grown onto substrates. The deposited layers are referred to as "epitaxial layers" or "epilayers". If the deposited crystal layer is a different material to the substrate, the process is referred to as heteroepitaxy. CBE is a form of epitaxial growth commonly used for III-IV semiconductor growth that involves gaseous sources and occurs under ultra high vacuum (UHV) [30]. The three main growth modes that occur in epitaxial growth are discussed in the preceding section on self-assembled nanoparticles, Section 2.4. This technique was first pioneered in the early 1980s [26], and has often been discussed as the more advantageous intersection of metalorganic chemical vapour deposition (MOCVD) and molecular beam epitaxy (MBE) [30].

Common gallium and indium based metalorganic compounds that make up the group III sources in CBE include triethylgallium (TEGa), trimethylgallium (TMGa), trimethylindium (TMIn), and triethylindium (TEIn). The group V sources are hydrides: highly toxic group V and hydrogen compounds such as arsine (AsH_3) and phosphine (PH_3). They are the easiest sources to control and the most pure and are therefore used despite their toxicity [30]. These sources are vapours under room temperature, and the crystal holder is usually heated to temperatures from 500-700°C [30].

Growth of InAs/InP nanoparticles can be performed using MBE, MOCVD, or CBE. CBE technique proves useful for III-V nanoparticle growth because it facilitates very fine tuning of deposited layer thicknesses, and also uses lower temperatures than MOCVD [30]. The growth rates in CBE are largely dependent on the group III flux, and are up to 1/hr [30].

3.1.2 Sample Descriptions

Ten different samples were studied using AFM. These samples were grown using a Riber 32P Reactor by chemical beam epitaxy (CBE) on InP substrates by Dr. Philip J. Poole at the National

Research Centre. The group III sources were pure TMIn and TEGa, and the group V sources were AsH₃ and PH₃. These sources were cracked - heated to high temperatures - before growth to form As₂ and P₂. Examples of the samples are shown in [3.1](#) alongside a description of the general layer structure.

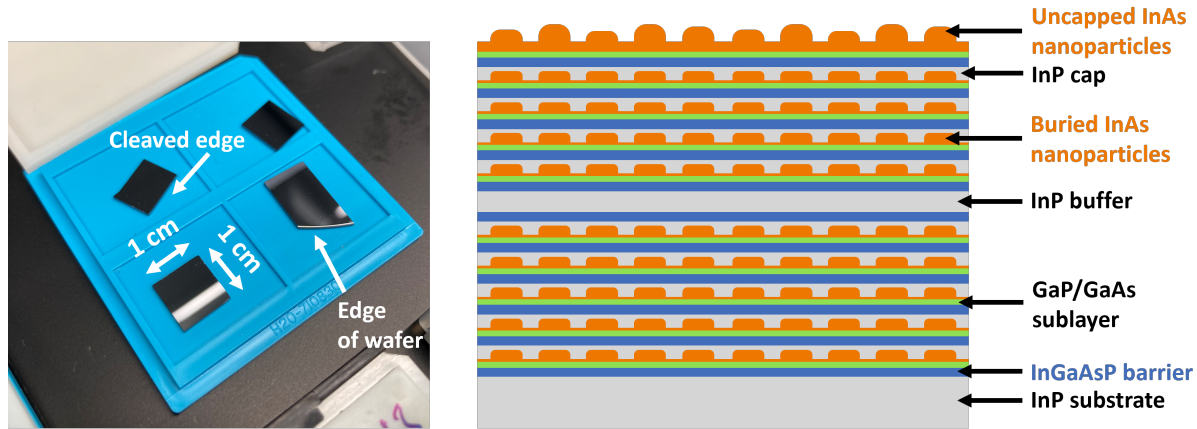


Figure 3.1: Image of four AFM nanoparticle samples showing cleaved and wafer edges (left); description of nanoparticle layer structure (right).

All ten samples are grown on InP substrates, with growth conditions outlined in Table [1](#). First, an InGaAsP quaternary is deposited onto an InP substrate. The composition of this quaternary is chosen such that it is lattice-matched to InP, and has a room temperature photoluminescence emission wavelength of 1.15 μ m. Then, a straining sublayer is deposited. For five of these samples this is GaAs with a nominal layer thickness of 0.44 nm, and for the other five it is GaP with a nominal layer thickness of 0.4 nm. InAs is then deposited to grow the self-assembled nanoparticles via the Stranski-Krastanow growth mode. To regulate the heights and cap the nanoparticles, InP is deposited in a double-capping process. This stack, from InGaAsP barrier to InP cap, is repeated for a total of 9 buried layers of nanoparticles: five layers, an InP buffer, and then four layers. The tenth layer is left uncapped and is analyzed using AFM. Quantum dash formation is enabled by lower arsenic overpressure, while doubling this overpressure leads to the formation of dots for the growth study samples. The deposition for GaAs sublayer samples was 12 seconds with a 20 second growth interruption, while faster growth rates of 8 seconds and a 20 second interruption was used for the GaP sublayer samples. From our collaborators at the National Research Council Canada, we were provided with room-temperature photoluminescence data for all ten samples.

Table 1: Nanoparticle sample information

Sublayer	Growth Temperature (°C)	PL Peak λ (to nearest nm)
GaP	500	1556
	510	1539
	520	1543
	530	1554
	540	1592
GaAs	500	1548
	510	1539
	520	1543
	530	1541
	540	1535

3.2 Atomic Force Microscopy

Atomic force microscopy is a high-resolution technique for probing the surfaces of microscopic devices. Unlike microscopy techniques that require light beams and focusing lenses, AFM can resolve beyond the diffraction limit since it instead uses a cantilever to detect micrometre and nanometre variations along a device surface. Traditional light microscopes cannot resolve the difference between the top surface of InAs nanoparticles or the wetting layer below them. Light imaging also cannot measure the height of these structures. AFM can solve both of these problems, making it the ideal technique for visualizing these structures. In addition, AFM traces the surface topography with nanometre precision, which is especially important since these nanoparticles are on the order of a few nanometres tall. Scanning electron microscopy (SEM) could also be used to image these nanoparticles, but the convenience of AFM data collection in terms of height variations measured by cantilever deflection still makes this technique preferable.

3.2.1 Procedure for AFM Image Acquisition

AFM measurements were performed at room temperature in ScanAsyst mode using Scanasyst-Air tips on a Bruker Dimension Icon AFM. These tips have silicon nitride triangular cantilevers and a nominal tip radius of 2 nm. Four images were taken per sample, with a scan size of $1\mu\text{m}^2$, a scan rate of 0.5 Hz, and a resolution of 1024 samples/line and 1024 lines/scan. Images were taken on four separate locations centred on the sample by raising the AFM head and manually changing positions, to ensure that the sites were indicative of the entire sample. The

sample was mounted such that the cantilever traced perpendicular to the longest lateral length of the nanoparticles. Post-image processing and analysis was performed with a combination of Python (version 3.9) and Gwyddion (version 2.59) on the height (zsensor) images to determine the heights, widths, and densities. As nanoparticles are capped with InP, they reduce in height and level out [31], thus it must be noted that the results from Table 2 are for uncapped InAs QDs/QDashes and will therefore differ slightly from buried QDs/QDashes grown with the same procedure and conditions.

To determine the average heights of the nanoparticles, the height distribution of each scan was extracted using Gwyddion. This data was then fitted using a three-term Gaussian. The difference between the peaks are then taken as the average heights. This process was repeated for all forty images. These heights were used to inform the layer thicknesses in the single QDash simulations outlined in the next section.

3.2.2 Procedure for Post-Processing of AFM Images

Standard Image Processing

1. Import AFM image into Gwyddion 2.59, released 2021-06-28
2. Level data by "mean plane subtraction"
3. Align rows using various methods: (1) Use polynomial fit with degree=1 to remove linear slopes within image. This subtracts the polynomial from each scan line of the image, therefore arranging each scan line to the same height.
4. Shift minimum data value to zero.
5. Correct horizontal scars on the image. During AFM analysis, the tip may produce artifacts that appears as "strokes" on the image - lines parallel to the direction of tip travel. These can be easily removed by the software.
6. Rotate image if necessary (an attempt was made to ensure that all images were taken such that the tip scanned perpendicular to the length of the QDashes. However, for some oval QD samples, the tip scanned parallel to some of the particles),
7. Calculate 1D statistical function: height distribution of scan. Ensure that entire 1024x1024 scan is selected, and export graph to a text file. Save this file as a .csv for ease of analysis in later stages.

8. Save the file as a scalable vector graphic to preserve the resolution. The files were saved with the following parameters:

Basic Parameters:

- (a) Pixel size = 0.1 mm
- (b) Pixels per inch: 254
- (c) Width 102.4 mm
- (d) Height 102.4 mm

Lateral Scale:

- (a) Inset scale bar, length 500 nm
9. If it is necessary to remove part of the dataset (dust, AFM artifact, etc.): Select interpolate small defects and manually select the smallest region necessary to remove. Perform this step after levelling the data, but before aligning the rows.

The procedure to extract the heights of nanoparticles is included in section 4.3 of this thesis. The average widths of the nanoparticles were estimated using the procedure outlined here. For density analysis, the nanoparticles were hand-counted.

Width Analysis

1. Once image is processed using "Standard Imaging Processing Procedure", use "extract profile along arbitrary line" tool to gather the height profiles across 25 nanoparticle widths. Exercise caution to ensure that cross-sections are taken as perpendicular to the longest dimension of the nanoparticle as possible.
2. After collecting 25 widths, "apply" the height profiles and save the resulting .csv file
3. For each of the produced data sets, calculate the FWHM of the resultant peaks. Then calculate the distance between these two points and use this as an estimation of the width of the nanoparticle. Then compute the average to get the estimated average nanoparticle width/scan image.
4. Complete this procedure for each AFM scan for a total of 100 widths/sample (4 scans/sample). The average of each of the four scans is then taken as the sample nanoparticle average width, with the standard deviation between the average scan width serving as the calculation uncertainty.

Density Analysis

1. Import processed SVG image into Gimp image post-processing or equivalent open-source post-processing software.
2. Manually trace all nanoparticles to estimate surface density of nanoparticles per scan.
3. Remove any nanoparticles intersecting with the right-hand vertical and upper horizontal edges to avoid oversampling.
4. The average nanoparticle density is taken between four scans/sample, with the standard deviation amongst the four samples serving as the uncertainty.

3.3 Energy Level Simulations

3.3.1 Description of Model

The model developed to simulate the emission wavelength and confined energy levels within single QDashes was created using Crosslight Photonic Integrated Circuit Simulation (PICS3D) software version 2020 [16]. PICS3D is a three-dimensional simulator that is ideal for simulating full laser structures. It was chosen for simulating single quantum dashes since the output files for these models can be easily implemented in macroscopic laser structures within the same program. This enabled the work in this thesis to be integrated into a full laser structure. This simulator is also useful as it allows the user to modify layer structures and devices with ease in all three dimensions.

The nanoparticle model included with PICS3D is a three-dimensional finite element method simulator, using single parabolic band models, anisotropic effective masses, and the stationary Schrödinger equation to solve for the band structure and energy levels within a customizable device structure [32]. The process is as follows: first, the user creates a layer structure in the .layer file(s), onto which a mesh is generated. The mesh can be adjusted according to user preference, and the process for selecting a mesh is described in Chapter 3.3.2. Once the desired mesh has been established, the simulation then solves for the band structure of the device using a parabolic band model. After the band structure is defined, the simulation initializes the quantum mechanical solver to solve the stationary Schrödinger equation at each mesh point to determine the subband energy levels and overlap integrals.

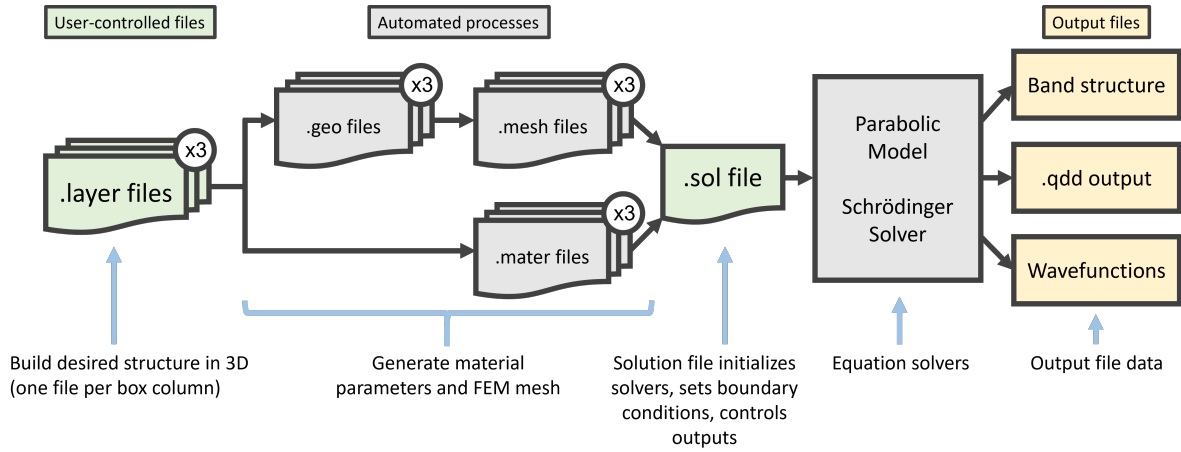


Figure 3.2: Flowchart describing process by which Crosslight builds a simulation project for an embedded QDash structure and what output files are produced. Further information about project setup can be found here [16]; this figure has been customized for the box-single model adaptation used for these simulations.

The model calculates transition energies and overlap integrals for three datasets: transitions between the (1) Γ conduction band valley subbands and the heavy hole valence subbands; (2) Γ conduction band valley and the light hole valence subbands; and (3) L conduction band valley subbands and the heavy hole valence subbands. For the purposes of these simulations, the first ten subbands in dataset (1) and (2) is considered, and the lowest energy transition between the first subband of the Γ and heavy hole band is taken as an estimation of the emission energy. The composition and structure of each individual layer can be varied to see the effect of all parameters on the energy transitions and spacing and thus the predicted emission wavelength.

This model has been adapted from Crosslight's box_single tutorial QDot model. This model is represented in cartesian coordinates, and is subdivided into three columns and three rows, where the inputs to all nine sections are individually controlled. This model is therefore ideal for simulating single quantum dashes as the length, width, and height of the dash can be modified independently. The full heterostructure consists of outer InGaAsP barriers (1.15Q), a GaP or GaAs sublayer (both are used experimentally for QDs or QDashes), an InAs_yP_{1-y} wetting layer and QDash, and an InP capping layer. The default layer thicknesses (i.e. the layer thickness when held constant in the simulation) are chosen based on literature review of similar structures and experimentally determined parameters.

To simulate each of these binaries, ternaries, or quaternaries, the In_{1-x}Ga_xAs_yP_{1-y} quaternary macro is implemented in Crosslight, which allows the user to use the same macro for each

layer, but vary the material by modifying x and y . It is called using the material library macro configuration, called *mater_lib*. This configuration makes it easy to switch between bulk and complex macro information by the presence of the *model = quantum_well* command. For our layer structure, all layers except the outer InGaAsP barriers are flagged with this model tag. Also contained in the macro information are the band offsets, bandgap equations, strain, and temperature effects. For the purposes of this thesis, the temperature is held constant at 300 K. The bulk bandgap offset ratio is set to 0.4, meaning that the conduction band offset:valence band offset ratio is 0.4:0.6. This is validated for the InAs/InP interface by [33]. This macro assumes that the material is strained to lattice-match an InP substrate [16]. The strain used for each segment of the layer structure is assumed constant throughout the entire segment, and is calculated using bulk lattice constant differences between InP and the material of the layer segment.

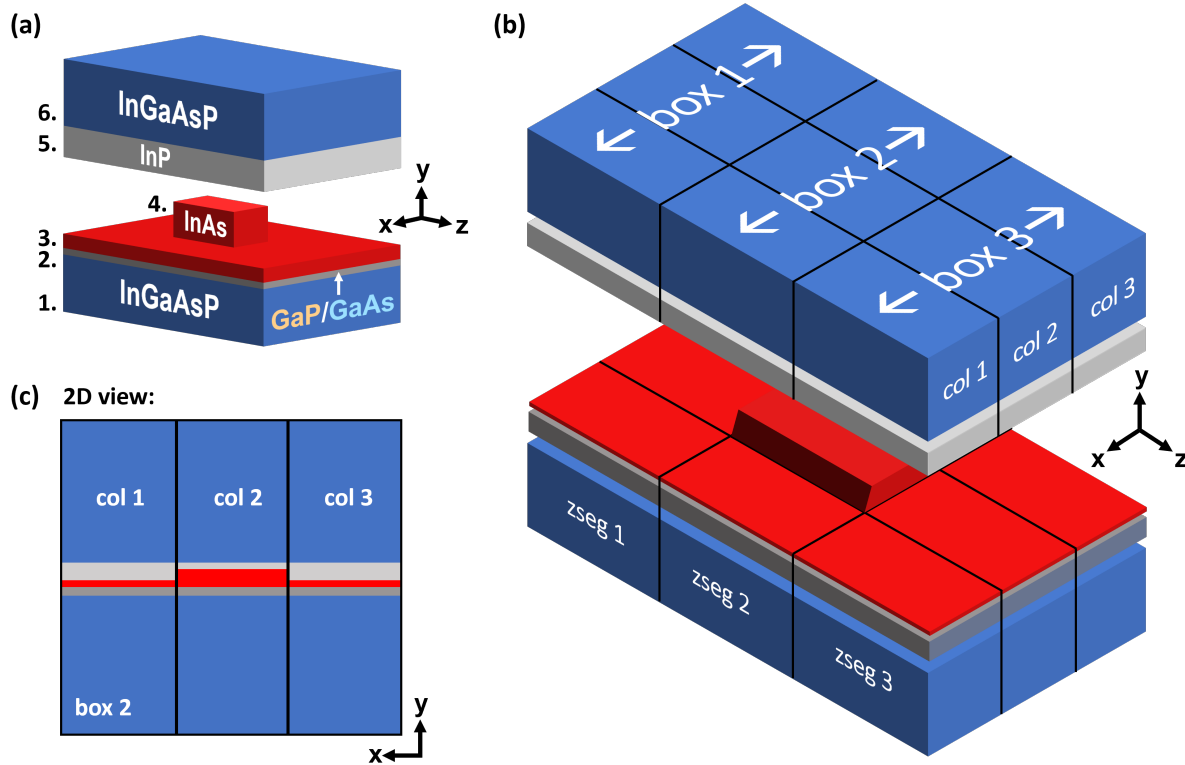


Figure 3.3: (a) Layer structure and material for single QDash simulation in exploded view; (b) Structure divisions for mesh and material allocation in exploded view; (c) 2D view of box 2 of heterostructure.

The boundary conditions within Crosslight can be controlled for each of the simulations edges, denoted as top, right, bottom, and left. These correspond to the four edges of the 2D view of

the structure in Fig. 3.4(c). An example of how to specify these boundary conditions within the solution file of the model is shown in the Appendix, section 8.3.2. This simulation uses Crosslight's Type 1 boundary conditions, which are referred to as Dirichlet boundary conditions [16]. This specifies that the wave intensity (in this case, the electronic wavefunction) must be zero at the zone boundary. Since the simulation has been designed with ample barriers both laterally and vertically to fully encase the QDash and confine the wavefunction, these boundary conditions are sufficient as they are intended for when the confined wavefunction is far away from the boundary.

3.3.2 Simulation Setup and Mesh Convergence

The mesh within a simulation defines the number and distribution of points where the simulation solves equations. A coarser mesh will give different results to a finer mesh and is more sensitive to incremental changes in mesh numbers. Determining an appropriate density for the mesh is therefore a crucial step when performing these simulations. Since the purpose of these simulations was to identify the relative changes to the emission wavelength and overlap integrals as a metric of confinement when varying layer thicknesses and compositions, if the established mesh were too coarse it would create a larger uncertainty between simulations. A mesh too coarse would not give enough resolution to capture necessary small changes in structure thicknesses, whereas a mesh too fine would lead to unnecessarily long computation times and simulation errors.

Our simulations were adapted from an example tutorial provided by Crosslight for single QDots in Cartesian coordinates. There are four variables which determine the density and distribution of the mesh: the vertical mesh lines controlled with *mesh_num*; the horizontal mesh lines per layer, *n*; the number of planes in the *z*-direction controlled with *zplanes*; and the mesh ratio controlling the distribution of mesh lines in both *x* and *y*, *r*. The mesh ratio is a ratio of the interval between adjacent mesh lines to the next interval: $r = \frac{\text{distance between mesh line } n \text{ and } n+1}{\text{distance between mesh line } n+1 \text{ and } n+2}$. A uniform mesh with uniform interval spacing thus occurs for $r = 1$. The mesh ratio r_y describes the distribution of mesh lines perpendicular to the *y*-axis and can be modified for each specified layer in the simulation. The mesh ratio r_x controls the distribution of mesh lines perpendicular to the *x*-axis, and can be specified for each column of the simulation. The mesh ratios utilized in simulations presented here, as well as the variables that control the mesh in Cartesian coordinates, can be found in Fig. 3.4.

For the active region, a mesh ratio of $r_y = 1$. was chosen to facilitate a homogeneous mesh

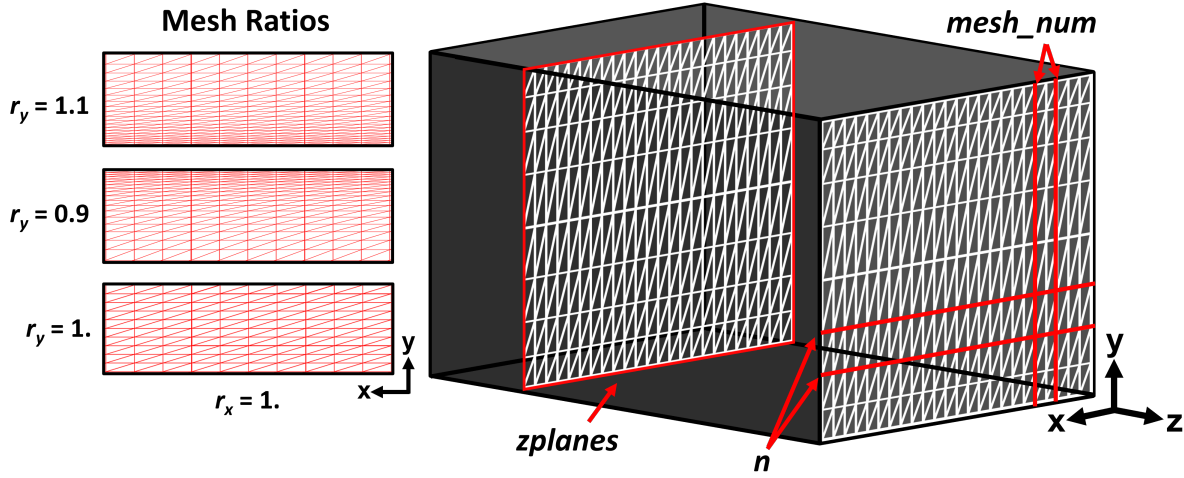


Figure 3.4: Summary of Crosslight variables that control the mesh in three-dimensional numerical simulations.

density throughout this heterostructure. To determine the number of mesh lines per layer and per column, we consider the physical meaning of the spacing. The thicknesses of each layer in the active region range from 0.1 to 2.5 nm; a mesh density in the y -direction of 1 Å per division was chosen so that the resolution was on the order of the smallest layer thickness. This was also the smallest possible division that could be selected, limited by the software and its error outputs. In the x -direction, the width of the QDash was varied by 5 nm increments when identifying the effect of QDash width on emission wavelength, and thus a mesh density of 2 nm per division was selected so that the resolution was approximately half of the change in width. A mesh ratio of either $r_y = 1.1$ or 0.9 was chosen for the outer InGaAsP (1.15Q) barriers so that the mesh density increased towards the active region of the heterostructure. These layers are considered bulk materials and the mesh is thus less important than within the active region.

The final mesh parameter, the number of *zplanes*, controls how many times the x - y mesh is iterated in a single box in the z -direction. Since this direction is the longest dimension of the QDash, it is expected that this will have the greatest impact on the energy level spacing of the subbands, rather than affecting the emission energy. Thus, to determine how many *zplanes* to use, it was increased until the energy levels of each subband were invariant to an additional increase in *zplane*.

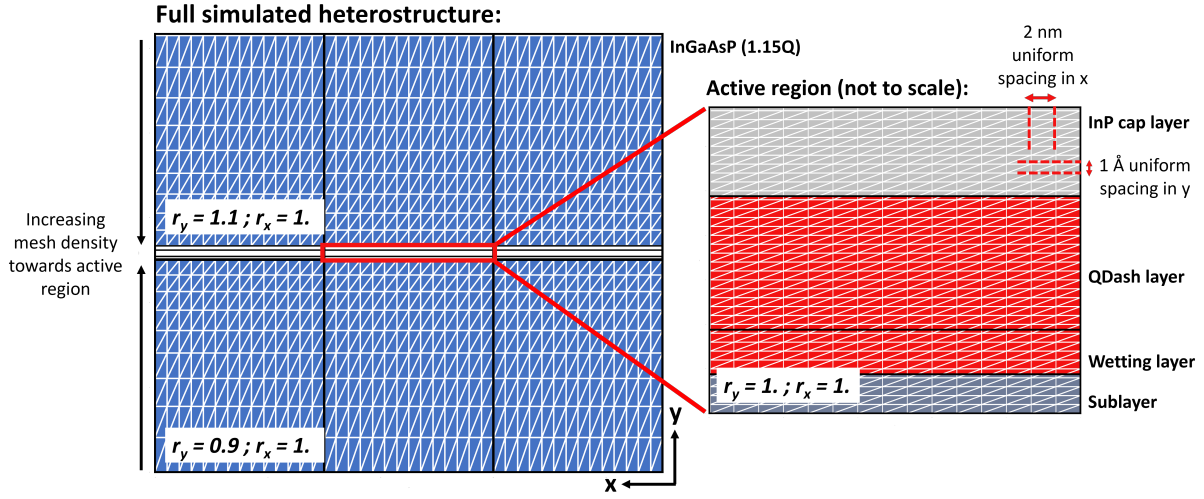


Figure 3.5: 2D x - y mesh for default simulation structure

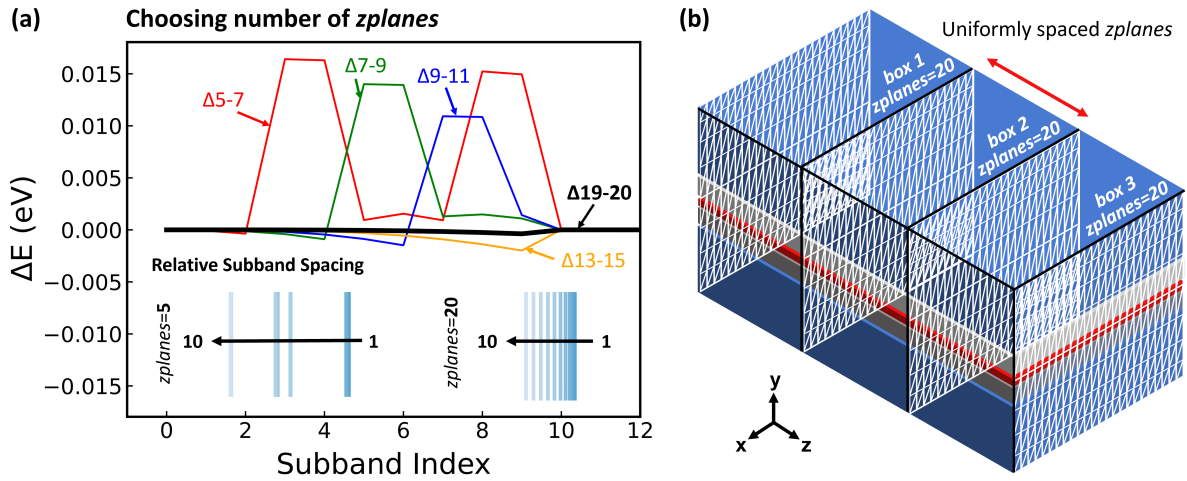


Figure 3.6: (a) Difference in energy levels between simulations with varying number of mesh planes, indicating that at 20 z planes there is minimal variation in energy level spacing and values when further changing the z mesh; (b) Visual description of x - y mesh iterated in z planes for full simulation structure

Chapter 4: Atomic Force Microscopy Experiments

4.1 Overview

A total of forty $1\text{ }\mu\text{m}^2$ AFM scans were performed, corresponding to four scans per sample. The uncertainties provided are the standard deviation in the respective variable between each of the four scans. One $2\text{ }\mu\text{m}^2$ image was taken for each sample. These scans were taken at 0.25 Hz scan rates and 1024×1024 resolution. A summary of the images is presented in Table 2, and all forty $1\text{ }\mu\text{m}^2$ images can be found in the Appendix.

Table 2: Average nanoparticle dimensions

Sublayer	Growth Temperature ($^{\circ}\text{C}$)	Maximum Height (nm)	Minimum Height (nm)	Width (nm)	Density (10^9 cm^{-2})
GaP	500	2.80 ± 0.7	1.29 ± 0.4	29 ± 7	37 ± 2
	510	2.98 ± 0.9	1.36 ± 0.5	29 ± 7	35 ± 3
	520	2.64 ± 0.1	0.93 ± 0.3	24 ± 4	37 ± 4
	530	2.50 ± 0.2	1.00 ± 0.6	30 ± 5	19 ± 0.3
	540	3.68 ± 0.3	1.15 ± 0.3	37 ± 4	23 ± 0.3
GaAs	500	2.20 ± 0.05	1.39 ± 0.3	32 ± 5	17 ± 1
	510	2.15 ± 0.04	1.28 ± 0.3	27 ± 5	15 ± 2
	520	2.36 ± 0.03	1.32 ± 0.2	28 ± 4	14 ± 3
	530	2.10 ± 0.2	1.24 ± 0.3	29 ± 5	10 ± 2
	540	2.26 ± 0.8	0.72 ± 0.6	36 ± 6	6 ± 0.9

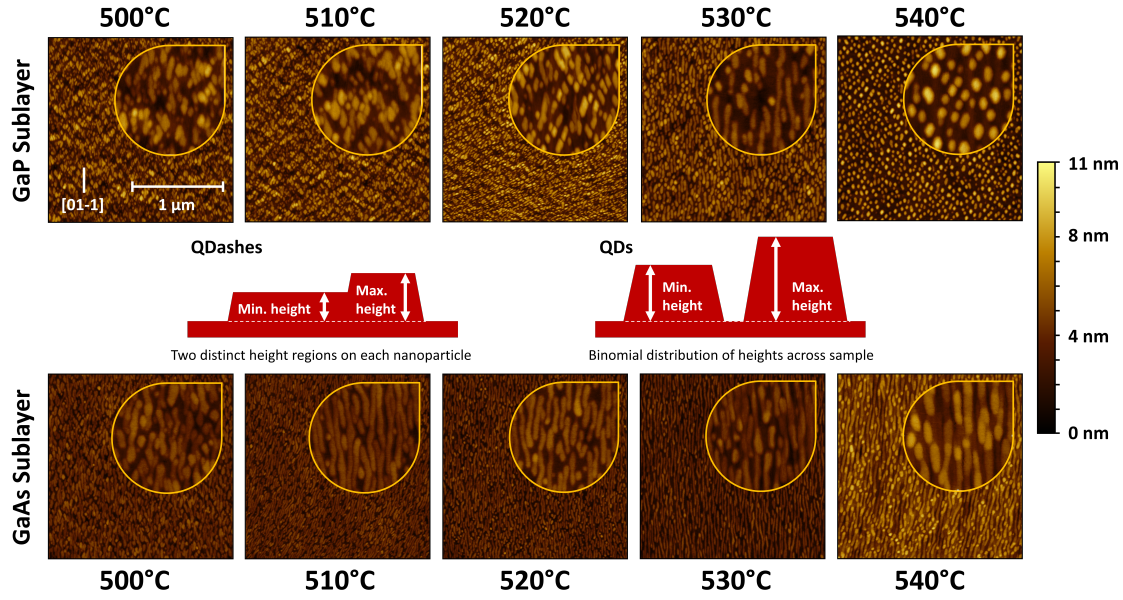


Figure 4.1: Summary of $2\ \mu\text{m}^2$ AFM images with insets showing zoomed-in nanoparticle structure. Centre insets describe the difference in height distributions for QDash and QD samples.

4.2 Preface and Author Contributions

This subsection contains our conference proceeding from Photonics West 2022, which was published through SPIE on March 28, 2022. This conference proceeding discusses the post-processing procedure of AFM images to determine the average heights of InAs/InGaAsP/InP uncapped QDashes. To the best of our knowledge, this is a novel procedure that utilizes the average height distribution of the entire AFM scan to extract peak and plateau QDash heights. The relationship between trends in uncapped QDash height and photoluminescence of capped QDashes for our particular samples is discussed. Measurements, analysis, and lead writing was performed by R-J. K. Obhi. Contributions from authors: S. W. Schaefer, advice, writing, and edits; C. E. Valdivia, advice and writing; P. J. Poole, sample growth and writing; J. R. Liu, conceptualization; Z. G. Lu, conceptualization; and K. Hinzner, conceptualization and writing.

4.3 Publication - Photonics West 2022

Ras-Jeevan K. Obhi, Sebastian W. Schaefer, Christopher E. Valdivia, Philip J. Poole, Jiaren Liu, Zhenguo Lu, and Karin Hinzer, "Height distributions of uncapped InAs/InGaAsP/InP quantum dashes and their effect on emission wavelengths," Proc. SPIE 12010, Photonics and Phononic Properties of Engineered Nanostructures XII, 120100C (5 March 2022); doi: 10.1117/12.2609954.

Height Distributions of Uncapped InAs/InGaAsP/InP Quantum Dashes and Their Effect on Emission Wavelengths

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ABSTRACT

The emission wavelength of self-assembled quantum dashes can be controlled by their height. Uncapped InAs/InGaAsP/InP quantum dashes are found to have two distinct heights, which we have measured with atomic force microscopy and denoted the plateau and the peak heights. These heights range from 0.50 nm to 2.35 nm. Under the same growth conditions, for increasing uncapped quantum dash heights we observe an increase in the photoluminescence peak emission wavelength from approximately 1535 to 1543 nm for the capped layers. A growth temperature of 520°C is determined to achieve uniform height distribution for 1550 nm emission using chemical beam epitaxy.

Keywords: quantum dot, quantum dash, quantum dash laser, atomic force microscopy, emission wavelength, epitaxy, Stranski-Krastanow growth

1. INTRODUCTION

Quantum dashes are short wire-like nanoparticles providing three-dimensional electron confinement that can be grown via the Stranski-Krastanow growth mode. The process of self-assembly using this mode for InAs quantum dots was first published in 1985 by Goldstein *et al.* [1]. This layer-plus-island growth, known as Stranski-Krastanow growth, is spontaneous due to the balance between surface energy and strain energy of the InAs layer [2], and requires a significant difference in lattice parameter between the substrate and the layer being grown. The growth mode is characterized by the initial two-dimensional growth of a wetting layer, a highly strained layer a few monolayers thick. After reaching critical thickness, islanding begins on top of the wetting layer to reduce the overall elastic energy of the system. InAs islanding is known to occur on both InP and InGaAsP and will preferentially form dashes or dots depending on the growth conditions. By capping these nanoparticles after self-assembly, quantum dash or dot arrays can be grown in stacks. These stacked arrays offer favourable properties as gain media in lasers compared to quantum wells when used to create multiwavelength lasers for high speed telecommunications [3]. Self-assembled InAs quantum dashes grown on InP substrates can be designed to emit at 1550 nm, in the C-band transmission band of optical fiber.

In this article, four InAs quantum dash samples are analyzed using atomic force microscopy (AFM) to determine the heights of uncapped surface dashes and the effect of growth procedures on dash formation. The method used to extract the heights of these uncapped dashes using open-source software is described, and the relationship between height of dashes and emission wavelength is established. Analyzing these samples yields valuable structural information to understand the confined electronic energy levels within these particles. This data has been used in single quantum dash simulations, which can in turn inform future growth processes and simulations for quantum dash lasers.

2. GROWTH OF QUANTUM DASH SAMPLES

2.1 InAs/InP self-assembled nanoparticles

InAs quantum dashes on InP substrates are grown by chemical beam epitaxy (CBE). The lattice parameter of InAs is 3.2% larger than InP, and thus Stranski-Krastanow growth readily occurs. As InAs is deposited on (001) InP the 2D to 3D transition occurs through the creation of elongated wire-like structures in the [01-1] direction [4]. With widths much shorter than their lengths, up to hundreds of nanometres, these wire-like nanoparticles are referred to as quantum dashes [4].

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Provided adequate growth interruption times, these dashes can separate into quantum dots with approximately equal lengths and widths. Other factors that affect InAs nanoparticle formation are the group V (As) overpressure, growth temperature, and surface orientation [4][5][6]. Approximately 2-5 monolayers of InAs form as the wetting layer [4]. Uncapped InAs quantum dots grown on InP substrates range from 5-15 nm tall depending on growth procedure and conditions, with widths from 15-40 nm and lengths upwards of 130 nm [4][7]. Quantum dashes can also exhibit taller peaks at the ends of the wires due to diffusion of material during growth interruption and sample cool down. When capped with InP to control their heights, buried InAs quantum dots exhibit heights typically ranging from 1.5-3 nm [4][8]. InAs dashes capped with InGaAsP have been reported with heights of approximately 2 nm [7][6][9][10]. Thin GaAs sublayers have also been deposited prior to the InAs wetting layer to encourage dash growth over dot formation [4]. InAs/InP quantum dot surface densities have been reported as high as $1 \times 10^{11} \text{ cm}^{-2}$ [4][11]. Heights and densities for InAs dashes on (100) InP substrates with varying buffer layer materials have been reported ranging from 0.4 to 3.1 nm and $10^9 - 10^{10} \text{ cm}^{-2}$, respectively [11].

2.2 Growth procedure of stacked InAs/InGaAsP/InP quantum dash samples

The quantum dash samples used in this study were grown by CBE with a Riber 32P reactor on n-type (001) InP substrates and consist of five stacks of quantum dash layers with the top layer left uncapped. The growth begins with deposition of an InP buffer followed by an InGaAsP quaternary lattice-matched to InP and emitting at 1.15 μm during room temperature photoluminescence measurements. After the InGaAsP layer a thin GaAs sublayer is grown to promote dash formation over dot formation. InAs is then deposited to form the dashes using a low As overpressure, followed by a 20 sec annealing step to allow some ripening of the dashes. The resulting structure after self-assembly is an InAs wetting layer with InAs dashes on top. InP is then used to encase the dashes in a double capping procedure involving a growth interruption between two deposition stages [4]. The InP fills the volume between the dashes, immersing the structures in InP, and the growth interruption serves to control the height distribution of buried dashes by allowing As/P exchange. The exact thickness of the wetting layer after capping is unknown, since As/P exchange will cause InP to form from the InAs wetting layer [4]. After dashes are capped with InP, an InGaAsP barrier is used again to vertically separate each layer of quantum dashes. The fifth and final quantum dash layer is left uncapped on the surface of the samples and was analyzed using AFM. A visual description of the samples is shown in Figure 1. For each sample the dash and barriers layers were grown at a different temperature ranging from 510°C to 540°C, modifying the dash formation and dimensions.

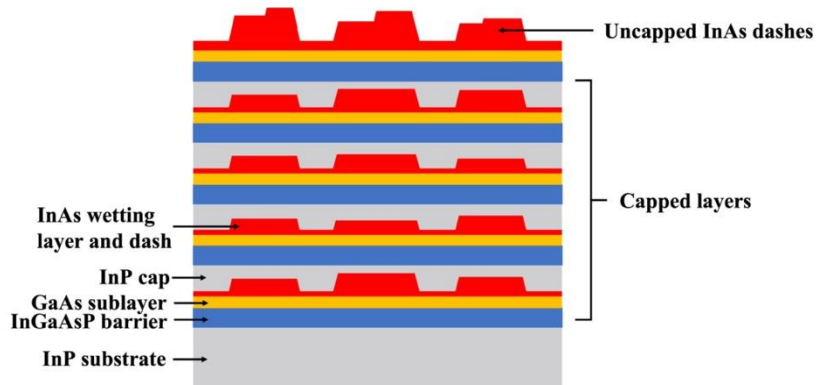


Figure 1. Description of layer structure for quantum dash samples with four capped layers and one uncapped dash layer at the sample surface. Grey: InP substrate and capping layers, blue: InGaAsP barrier layers, yellow: GaAs sublayer, red: InAs wetting layers and dash layers.

3. STRUCTURAL ANALYSIS OF QUANTUM DASH SAMPLES

3.1 Measurement and analysis approach

Atomic force microscopy measurements performed using a Bruker Dimension Icon AFM were used to analyze the uncapped InAs quantum dash samples. Four scans at different regions of the sample separated by millimetres were taken to enable averaging that will better characterize the entire sample. Examples of one image taken for each sample are shown in Figure 2. The outer edge of the substrate was avoided since morphology and dash density is impacted by proximity to the edge. The scan conditions are outlined in Table 1.

Table 1. Parameters used for AFM image capture

AFM Parameter	Details
Scan edge size	1 μm
Scan resolution	1024 $\times$ 1024
Scan rate	0.5 Hz
AFM Mode	Tapping (ScanAsyst)
AFM cantilever	ScanAsyst-Air tips: silicon nitride triangular cantilevers
Nominal tip radius	2 nm

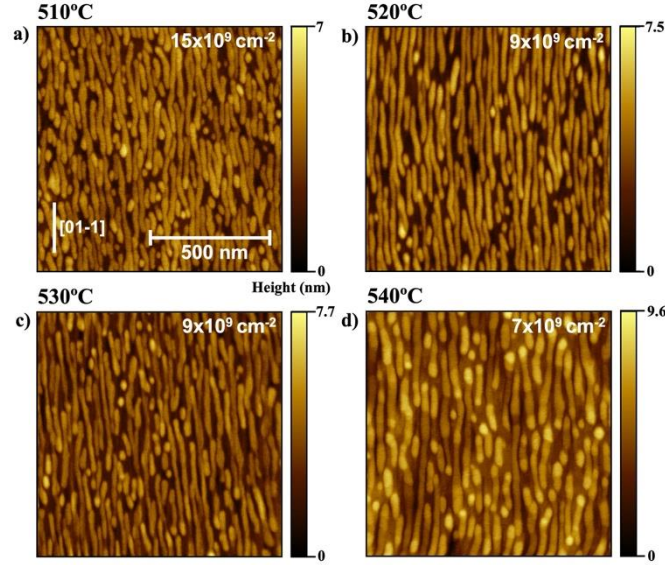


Figure 2. Example AFM images of each quantum dash sample at a) 510°C, b) 520°C, c) 530°C, d) 540°C. Images are 1 μm^2 and direction of dash elongation is indicated. Approximated dash densities are listed at the top right of each image.

All AFM images were analyzed using the same process in the open-source software Gwyddion [12]. Data was levelled using mean plane subtraction and a first order polynomial was used to remove linear slopes and arrange each scan line to the same height. The minimum data points were then shifted to zero to establish a baseline. Approximated dash densities were extracted by examining four out of the sixteen AFM images, yielding densities of 7 – 15 $\times 10^9 \text{ cm}^{-2}$ which is on the order of literature values for dash densities and lower than InAs/InGaAsP/InP dot densities [11][4].

Height distributions were extracted from each scan using the one-dimensional statistical function and then fitted using a three-term Gaussian. An example distribution and the corresponding Gaussian terms are shown in Figure 3a, where ρ is the probability density such that $\int_{-\infty}^{\infty} \rho(h)dh = 1$ where h is the height [12]. The first Gaussian term (I) represents the average height distribution of the background area between dashes, which corresponds to the surface roughness of the wetting layer; the second term (II) is the average height distribution of the plateau of the dashes; and the third term (III) is the average height distribution of the local peaks on the dashes arising due to material accumulation at the ends of the dashes during the self-assembly growth process. These three regions are labelled in an example AFM scan in Figure 3b and illustrated diagrammatically in Figure 3c. To determine the mean plateau and peak dash heights of a single scan, the difference between the Gaussian maxima of terms (II) and (I), and (III) and (I) were taken, respectively.

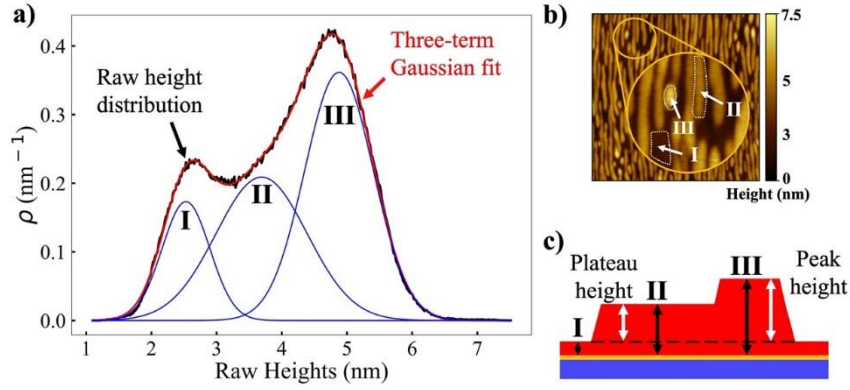


Figure 3. a) Black curve: raw height distribution of single AFM image; red curve: three-term Gaussian fit of raw height distribution; blue curves: individual three Gaussian terms extracted from red curve; b) AFM image with labels corresponding to each height region of the sample; c) visual representation of side profile of surface quantum dash, white arrows indicate dash plateau height and peak dash height.

3.2 Growth temperature and dash height

Measurements demonstrate that varying the growth temperature from 510 to 540°C causes variations in the peak dash height of almost 0.5 nm. Table 2 lists the plateau and peak heights for each sample averaged from four scans. Figure 4 graphically represents the average (a) plateau and (b) peak heights in grey, with black error bars corresponding to the maximum and minimum values from the four scans. The plateau height has larger variations between each scan on a single sample surface. As growth temperature reaches 540°C, the average plateau height decreases by approximately 0.5 nm and the surface density of dashes is low compared to other growth temperatures. From Figure 4 we see that the optimal temperature range to grow dashes with the least height variation across four scans is 520°C. This is desirable since the height is used to tune the emission wavelength, and dash layer uniformity is associated with increased optical gain [13].

Table 2. Growth temperature for quantum dash samples with GaAs sublayer and average heights of uncapped dashes

Temperature (°C)	Average Plateau Height (nm)	Average Peak Height (nm)
510	1.14	2.13
520	1.42	2.35
530	1.24	2.10
540	0.50	1.89

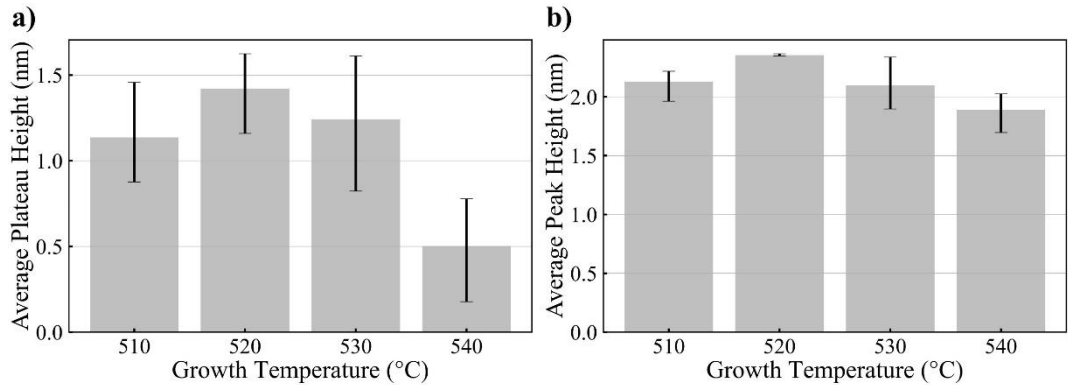


Figure 4. Graphical representation of a) average plateau heights and b) average peak heights of uncapped InAs/InGaAsP/InP quantum dashes. Grey bars indicate average value of height from four different images, and error bars indicate maximum and minimum heights across the four images.

3.3 Plateau height and emission wavelength

The lateral dimensions of these quantum dashes are much larger than their heights, therefore energy confinement primarily occurs in the growth direction and determines the nanostructure emission wavelengths [4]. The room temperature photoluminescence emission wavelengths of the four samples are shown in Figure 5a. A growth temperature of 520°C yields the tallest peak and plateau dashes and also corresponds to the emission wavelength closest to the target 1550 nm range. We observe that the relationship between plateau heights and room temperature photoluminescence emission wavelength of the capped dashes is linear for the samples considered. This is shown in Figure 5b.

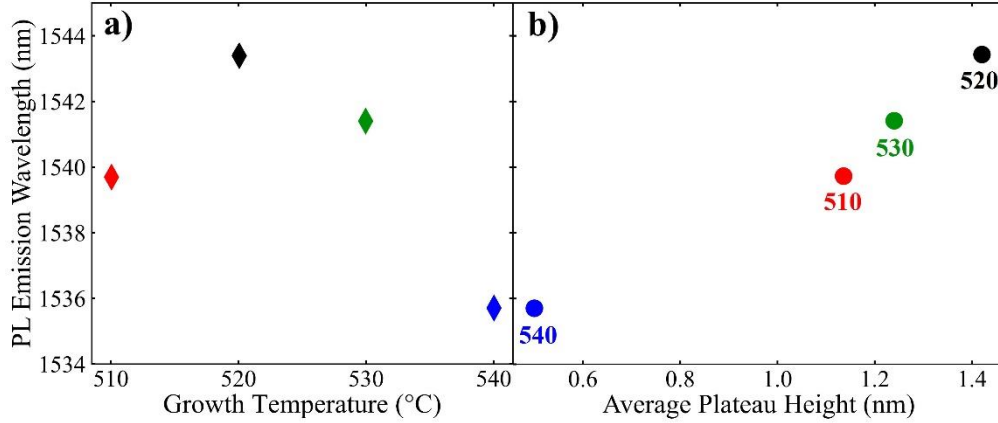


Figure 5. Room temperature photoluminescence emission wavelength of capped quantum dash layers a) as a function of growth temperature and b) as a function of average plateau height with temperature indicated for each data point.

4. SUMMARY

Uncapped InAs/InGaAsP/InP quantum dashes were investigated by performing image analysis on AFM scans. There are two distinct height regions identified on these nanoparticles using Gaussian fitting, with one Gaussian distribution corresponding to the elongated plateau of the dashes and another to the peak of the dashes that arises due to surface diffusion dynamics. The optimal temperature range in which to grow uniform dashes emitting closest to 1550 nm is found to be 520°C for the samples considered. This corresponds to the tallest dashes of the samples investigated for both plateau and peak heights. Average peak heights range from 1.89 nm to 2.35 nm. Average plateau heights under 540°C are found to range from 1.14 to 1.42 nm. A growth temperature of 540°C is found to noticeably decrease dash density, plateau, and peak heights, and thus emission wavelength. Since quantum dashes break up and collect to form dots in the Stranski-Krastanow growth mode, they are expected to be thinner than quantum dots. These heights are therefore comparable with similar InAs/InGaAsP/InP nanoparticles in the literature [4][7][11]. The capped quantum dashes in these samples are expected to be shorter than the peak heights identified in this paper due to the InP capping process. The average heights of the dashes extracted from these scans are used to inform the dimensions of single quantum dash simulations investigating the effect of quantum dash structure and composition on emission wavelength.

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Chapter 5: Single Quantum Dash Simulations

5.1 Preface and Author Contributions

This subsection contains a manuscript submitted to Applied Physics Letters in November 2022. The letter contains further AFM analysis including densities and widths of the nanoparticles that are outlined in Table 2. Single QDash simulations are used to investigate the effect of sub-layer type and phosphorus concentration within the QDash and WL on the band diagram and confined energy levels of the layer structure. The article concludes that GaAs sublayers and QDash heights from 1.5 to 2.0 nm will emit at approximately 1550 nm, and that phosphorus concentration arising from the documented As/P exchange process between InAs nanoparticles and InP capping layers can be used to further tune the emission wavelength. Simulations, measurements, and lead writing performed by R-J. K. Obhi. Contributions from authors: S. W. Schaefer, advice and edits; C. E. Valdivia, writing; J. R. Liu conceptualization; Z. G. Lu, conceptualization; P. J. Poole, sample growth and writing; and K. Hinzer, conceptualization and writing.

5.2 Publication - Submitted November 2022

Ras-Jeevan K. Obhi, Sebastian W. Schaefer, Christopher E. Valdivia, Jiaren Liu, Zhenguo Lu, Philip J. Poole, and Karin Hinzer, "Indium arsenide single quantum dash morphology and composition for wavelength tuning in quantum dash lasers", submitted November 2022 to Applied Physics Letters.

Indium arsenide single quantum dash morphology and composition for wavelength tuning in quantum dash lasers

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(Dated: 20 December 2022)

InAs quantum dot and dash gain media demonstrate performance benefits such as lower threshold current densities and reduced temperature sensitivity over quantum wells for lasers operating in the C-band telecommunications window. Quantum dashes are of much interest for their higher gain over quantum dots due to an increased density of states. We combine experimental results and simulations to understand how quantum dash morphology and composition can be used to tune the emission wavelengths of these nanoparticles. AFM analysis is performed to determine the effect of growth temperature and sublayer type on InAs/InGaAsP/InP nanoparticle morphology and homogeneity. Uncapped InAs nanoparticles grown by CBE on a GaAs sublayer will have dash-like geometries with heights up to 2.36 nm for growth temperatures of 500-540°C. GaP sublayers will induce taller quantum dots except for a growth temperature of 530°C, where quantum dashes form. The dimensions extracted from AFM scans are used in conjunction with photoluminescence data to guide parabolic band simulations of an InAs quantum dash with a GaP or GaAs sublayer and InP cap buried within InGaAsP. The calculated emission energy of a buried 30×300 nm quantum dash decreases by ~100 meV for increasing heights from 1.5 to 2.5 nm, or increases by ~100 meV by addition of 20% phosphorus in the dash and wetting layers. Modifying the quantum dash height and leveraging the As/P intermixing that occurs between the InAs and InP layers are thus most effective for wavelength tuning.

InAs/InGaAsP/InP quantum dots (QDots) and quantum dashes (QDashes) can be used as the active media in telecommunications lasers^{1,2} to offer improved device performance when compared to equivalent quantum well (QW) devices³⁻⁵. We define QDots as nanoparticles with lateral dimensions on the same order of tens of nanometers, and QDashes as those with one elongated lateral dimension on the order of hundreds of nanometers. The InAs/InP material system, with a lattice mismatch of 3.2%, enables either QDash or QDot growth depending on growth conditions and sublayer type. Both InGaAsP⁶ and InAlGaAs⁷ barriers can be implemented for C-band operation. Wavelength tuning via QDash height for InAs/InAlGaAs/InP QDash lasers has been well-documented^{8,9}. InAs/InGaAsP/InP QDash lasers, with lower strain than InAlGaAs, were the first to be demonstrated for use in optical communications^{8,10}.

Previous experiments have investigated the composition and structure of InAs QDash arrays with atomic force microscopy (AFM), photoluminescence (PL), cross-sectional scanning tunnelling spectroscopy, and transmission electron microscopy¹¹⁻¹⁵. The effect of parameters such as growth temperature and indium flow have been discussed for buried and uncapped nanoparticles. QDash simulations^{12,16-19} investigated the effect of QDash structure on emission and gain characteristics¹⁶⁻¹⁸, energy levels^{16,17}, and density of states of QDashes^{12,19} and their relation to other nanoparticles like quantum wires (QWires)^{12,18,19}. Both simulations and experiments characterized InAs nanoparticles on InP and GaAs substrates, showing that: QDashes facilitate wavelength tuning with their broader gain spectra than QWs¹⁹; QDashes have

QWire-like characteristics^{12,17}; and emission characteristics of QDashes are generally independent of QDash length^{16,17}.

This letter analyzes an asymmetric heterostructure with thin GaP and GaAs sublayers using experiments and simulations. While both uncapped QDot and QDash arrays are analyzed experimentally using AFM, we focus our modelling on QDashes due to their higher optical gain compared to QDot devices¹⁸. These single QDash energy level calculations were performed to understand the impact of morphology and composition on the predicted emission energy of QDashes, for telecommunications laser active media. The simulated heterostructure consists of InGaAsP barriers lattice-matched to InP, GaP or GaAs sublayer, InAs wetting layer (WL), InAs QDash, and InP cap. The QDash is designed to emit at 1550 nm in the C-band telecommunications window, and reproduces the structure of experimental growths of QDash arrays for InP-based lasers. The effect of As/P intermixing between the InP and InAs layers is considered by simulating the inclusion of phosphorus in the QDash and WL.

Ten InAs/InGaAsP/InP nanoparticle samples were grown by chemical beam epitaxy on n-type (001) InP substrates using a Riber 32P reactor. Example AFM scans of the uncapped nanoparticles are shown in Fig. 1(a)-(j), with the full structure shown in Fig. 1(k). Further growth information is included in the supplementary information. Since both GaP and GaAs sublayers will impact the resulting nanostructure morphology²⁰, five samples with growth temperatures from 500-540°C were analyzed for each sublayer type. Both sublayers reduce As/P exchange between the InAs and lower InGaAsP layers^{20,21}. GaP has the highest bond strength of the

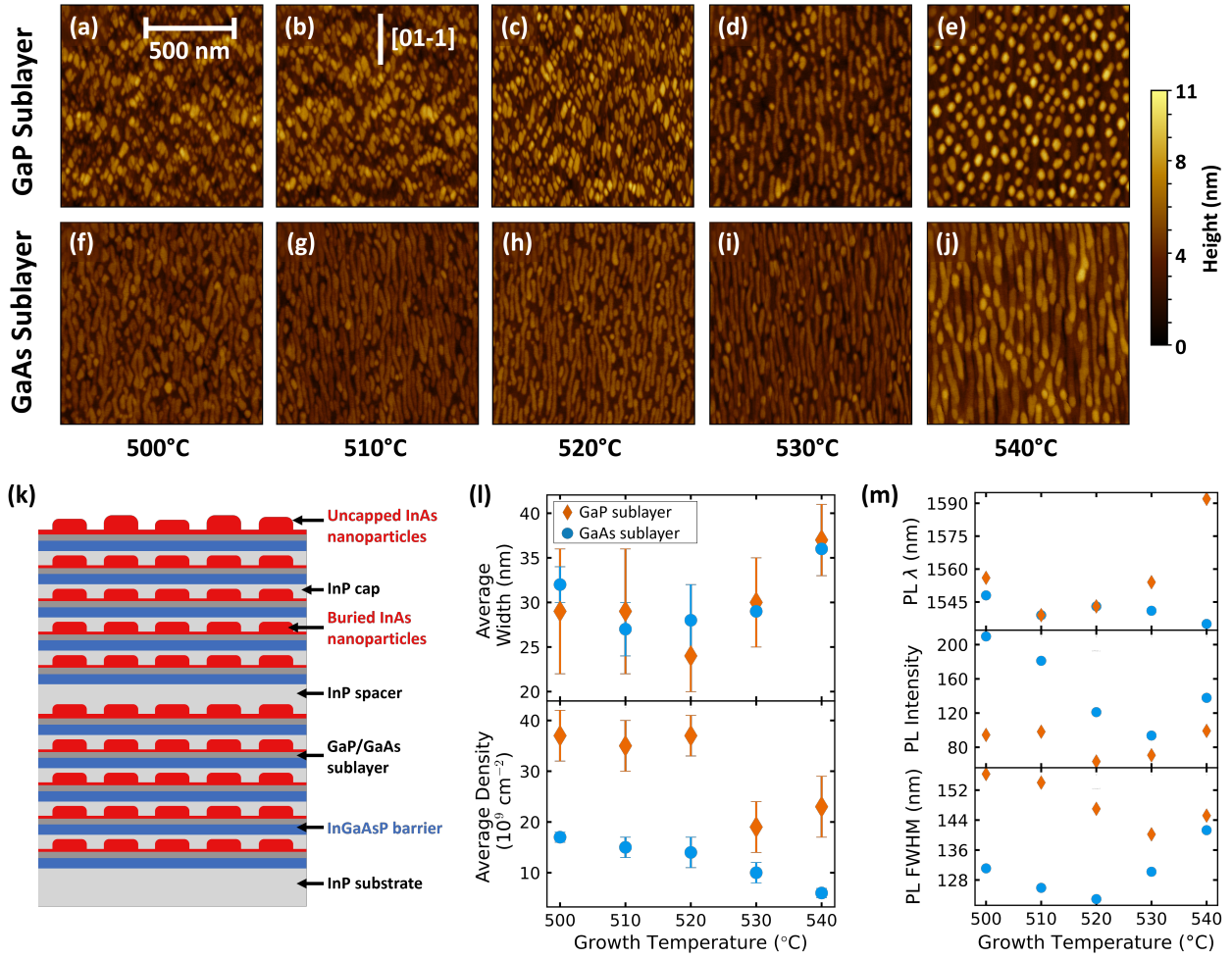


FIG. 1. (a)-(j) Single scan of ten samples analyzed using AFM. Each scan is $1 \mu\text{m}^2$ with vertical axis oriented in [01-1] direction. Samples (a)-(e) are grown on GaP sublayers, samples (f)-(j) on GaAs sublayers under different growth temperatures; (k) Description of sample layer structure; (l) Average nanoparticle widths and densities; (m) Room temperature PL data as a function of growth temperature.

InGaAsP compositions, making it energetically unfavourable for As/P exchange to occur. With GaAs, there is no phosphorus to exchange with arsenic. GaAs sublayers of monolayer thicknesses or less have also been shown to induce QDash formation in the [01-1] direction due to preferential surface diffusion^{9,20}.

Four AFM scans per sample were performed using a Bruker Dimension Icon AFM. The average nanoparticle widths and surface densities are shown in Fig. 1(l), with error bars showing the standard deviation across the four scans. The lowest density, shown in Fig. 1(j), corresponds to ~ 60 QDashes/ μm^2 , while the largest in Fig. 1(c) is ~ 360 nanoparticles/ μm^2 . As growth temperature increases, the average density for GaAs sublayer samples decreases, whereas for GaP there is a minimum density at 530°C. Average widths were taken for 100 nanoparticles for each sample, or 25 nanoparticles per scan. These values correspond well to literature values within the same material system^{9,12,22}. Room temperature PL data for the center wavelength, peak intensity, and full-width-half-maxima (FWHM) are shown in Fig. 1(m). The GaAs sub-

layers, which preferentially form QDashes instead of QDots, have higher PL intensities and lower FWHM, thus showing higher material gain than GaP sublayer samples at equivalent growth temperatures. In addition to sublayer type, arsenic and phosphorus overpressures and interruption times¹³, growth temperature^{13,23}, element intermixing^{24,25}, and surface diffusion dynamics^{20,26} all affect the morphology and composition of the nanoparticles. Over the range of temperatures considered here, GaAs sublayers produce QDashes, while GaP sublayers produce QDots with exception of 530°C, where QDashes are visible in Fig. 1(d).

Height probability distributions from all forty images were extracted using the data visualization and analysis open-source software, Gwyddion, and fitted with a three-term Gaussian as shown in Fig. 2(a) and (b). Exemplary regions corresponding to each of the three heights are outlined visually in Fig. 2(c) and (d). For all samples, peak (i) corresponds to the background height distribution (WL surface). For QDashes, peaks (ii) and (iii) correspond to primary plateaus and secondary peak heights of the QDashes, respectively.

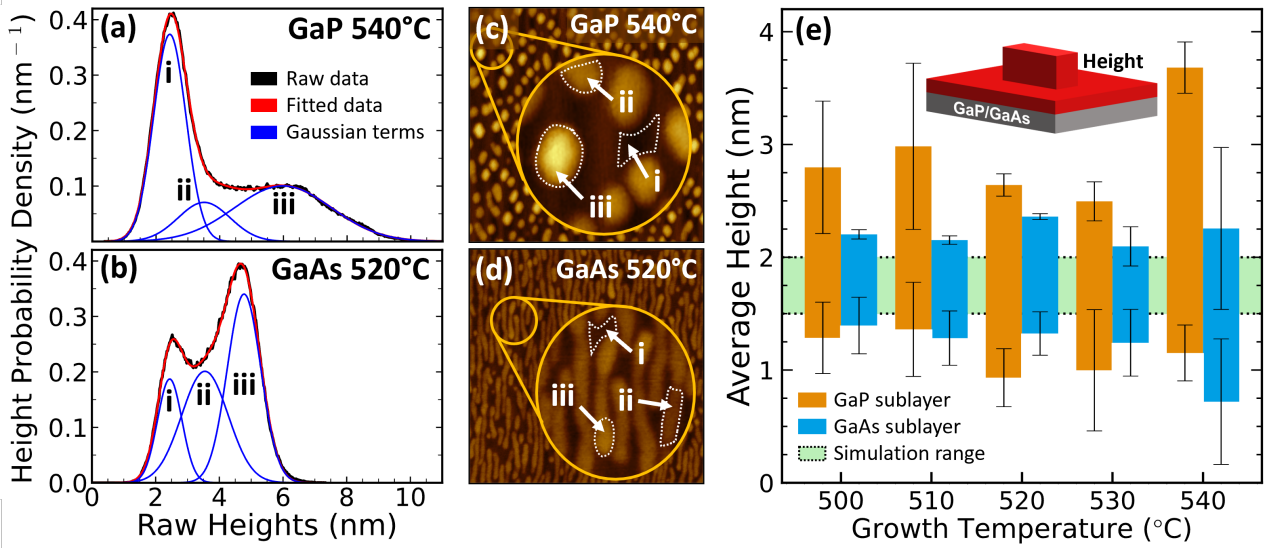


FIG. 2. Example height probability distributions with three Gaussian terms for (a) GaP and (b) GaAs sublayer with corresponding regions on AFM scans for (c) 540°C GaP and (d) 520°C GaAs samples; (e) Average minimum and maximum heights for each growth temperature from four scans.

TABLE I. Material parameters for default simulation structure

Layer	Thickness ^a (nm)	Phosphorus (%)	Strain ^b (%)	Effective Electron Mass
6. InGaAsP	50	-	0	0.07 m_0
5. InP cap	1	-	0	0.08 m_0
4. InAsP QDash	1.5 (1.5-2.5)	0 to 20	-3.2 to -2.5	0.023m_0 to 0.035 m_0
3. InAsP WL	0.5	0 to 20	-3.2 to -2.5	0.023m_0 to 0.035 m_0
2. GaP/GaAs sublayer	0.4/0.44 (0.1-1.0)	-	7.1/3.6	0.170 m_0 /0.064 m_0
1. InGaAsP	50	-	0	0.07 m_0

^a values in parentheses indicate simulated range

^b negative indicates compressive strain, bold indicates strain for 0% phosphorus condition

For InAs QDots, it is common to form a bimodal height distribution²⁷⁻³⁰, and thus peaks (ii) and (iii) correspond to the shorter and taller ensembles. The full AFM height analysis procedure is described and explained in Obhi et al.³¹. The minimum and maximum heights shown in Fig. 2(e) are the differences between the peaks of terms (i) and (ii), or (i) and (iii), respectively. This shows that uncapped nanoparticles on GaAs sublayers can grow to nearly 2.5 nm. The InP capping process reduces the height of nanoparticles²⁴, so simulations where QDash height is fixed are performed for heights of 1.5 or 2 nm, indicated by the green shaded region.

Three-dimensional energy level calculations of single QDashes were performed using the commercial optoelectronic simulation platform Crosslight Photonic Integrated Circuit Simulation (PICS3D)³². These simulations compute the band structure of the device described in Fig. 3 and Table I using a single band parabolic model with anisotropic effective heavy hole and light hole masses to account for strain effects. The effective electron masses are for the Γ valley and are given in Table I. The single band parabolic model has been validated in previous quantum structure simulations to determine energy level spacings^{16,17,19,33}. The finite element

mesh density is fixed at 1 Å spacing along y for layers 2-5, corresponding to the region containing the bulk of the carrier probability. The simulation solves the locally discretized stationary Schrödinger equation to obtain wavefunctions and eigenenergies at each mesh point. The ground state transition, from the Γ point of the first conduction band (CB) subband and the first subband of the heavy hole valence band (VB), is the lowest energy transition and is taken as the expected emission wavelength, although the simulation outputs up to ten confined levels in the CB and VB. The strains listed in Table I are calculated for lattice-matching to InP using bulk lattice constants and are constant throughout each material element. The simulated emission wavelength of the default 1.5 nm InAs QDash and WL with GaAs sublayer is tuned to 1549 nm to match experimental PL data shown in Fig. 1(m). This was done by modifying the barrier mesh and WL thickness while maintaining default structure dimensions from Table I.

The simulated heterostructure is shown in Fig. 3(a). As shown by the band diagrams in Fig. 3(b) and (c), the carrier confinement due to band offsets with a GaP sublayer is much deeper than for GaAs. To identify the effect of QDash composition on the bandgap, an increase from 0-20% phos-

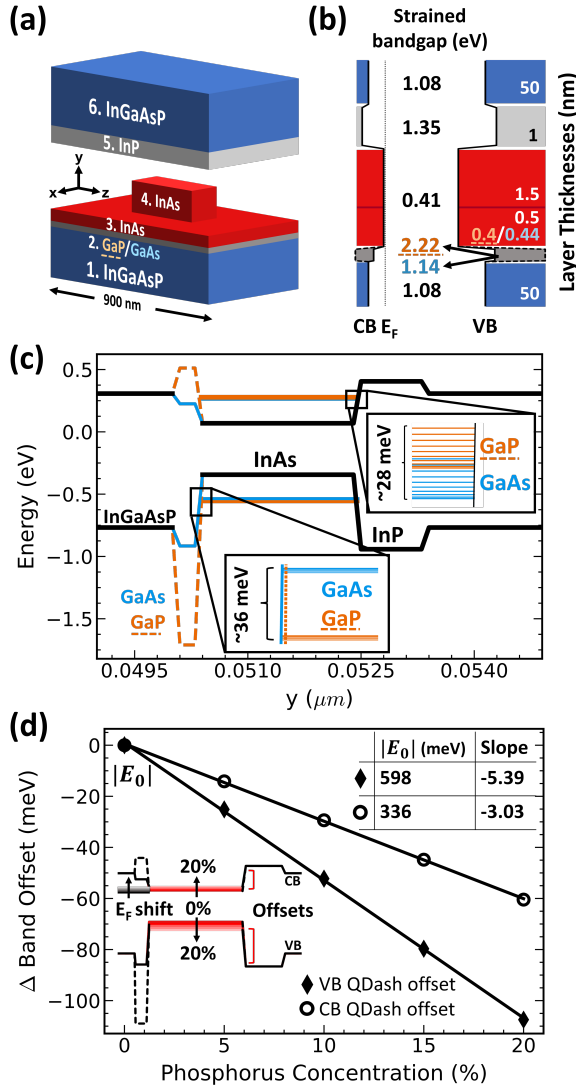


FIG. 3. (a) Exploded view of simulation structure; (b) Equilibrium bandgap diagram at 300 K, with Fermi energy (E_F) as indicated; (c) QDash conduction and heavy hole band diagram, with insets showing energy levels within $1.5 \times 30 \times 300$ nm QDash for GaP and GaAs sublayers; (d) Magnitude change in bandgap offsets as a function of [P] within QDash and WL, with reference $|E_0|$ defined as offset for 0% P. Inset table and figure: offset and band shift between QDash and InP cap for 0-20% phosphorus and slope of linear fits.

phorus concentration, [P], was applied to both the QDash and WL, which increases the bandgap as shown in Fig. 3(d). The band offsets in this plot refer to the junction between the InAs QDash and InP capping layer. The CB/VB offset ratio at this interface for a pure InAs QDash calculated using Crosslight material parameters is 34/66, corresponding well to the Piprek et al. value of 40/60 for the InGaAsP/InP material system³⁴.

Fig. 4 describes the effect of QDash dimensional changes on the emission energy for both GaAs and GaP sublayers. The solid lines represent a pure InAs QDash and WL, while dashed lines represent an inclusion of [P] = 10% in the QDash and WL. All lines are exponential fits of the form $y = Ae^{-bx} + c$,

where A, b, and c are freely chosen fit parameters. The fit residuals are small, with $R^2 > 0.995$. Fig. 4(a) shows that the emission energy as a function of QDash length converges for a QDash length of ~ 200 nm, and so a QDash length of 300 nm was chosen to remove the transition energy dependence on this dimension for simulations where the length is fixed. The rate of change in emission energy as a function of QDash width is shown in Fig. 4(b). There is also an exponential decay which converges at ~ 85 nm. We chose a QDash width of 30 nm for all simulations as all ten studied samples had nanoparticles with widths or diameters equal to this value, within standard deviation limits. While the effect of QDash dimensions has been previously investigated, we have included the impact of QDash and WL composition in tandem with changing QDash dimensions. There is negligible difference in the convergence of the emission energy with length or width between sublayer type or QDash composition, validating that the first transition emission energy is largely dependent on the smallest dimension, the vertical confinement.

As shown in Fig. 4(c), increasing the height of the QDashes from 1.5 - 2.5 nm decreases the emission energy exponentially by approximately 80 to 115 meV. A visual representation of this QDash height is given in Fig. 4(d). This trend has also been documented in Gioannini¹⁷, with a similar shift in energy for the same QDash heights. We have also investigated the effect of sublayer type and [P] on this parameter: GaP sublayers induce a larger change in emission energy, and including 10% [P] reduces the change in emission energy due to decreased band offsets shown in Fig. 3(d). The wavelength of the transition at a QDash height of 1.5 nm, labelled the initial wavelength λ_0 , is shown in Fig. 4(e). For QDash heights of 2.5 nm on a GaAs sublayer, the emission wavelength is pushed beyond the C-band telecommunications window, validating that shorter QDash heights such as those measured via AFM are better suited for 1550 nm emission. Experimental and calculated analysis of InAs/InP QWs by Kobayashi et al. have shown a similar trend for emission energy as a function of InAs well thickness, where on the same length scale, the trend is also sublinear³⁵. In Kobayashi's study, an increase of InAs QW thickness from 1 to 5 monolayers decreased the emission energy by ~ 300 meV. This corresponds to ~ 1 nm increase in thickness, the same delta across our studied range of QDash heights.

Next we consider the effect of sublayer type on the emission energies. As expected, the deeper confinement from GaP due to the larger bandgap and offsets results in higher emission energies. A higher bandgap barrier material also increases the effect of QDash height on energy level spacing: the rate of emission energy decrease with QDash height for GaP sublayers is higher than for GaAs sublayers. An increase of 10% [P] within the QDash and WL decreases the initial emission wavelength by approximately 80-90 nm for GaP and GaAs sublayers, respectively, and decreases the sensitivity of emission energy on QDash height. This is due to increasing [P] lowering the compressive strain and decreasing both the VB and CB offset, as shown in Fig. 3(d). Varying the height of a QDash from 1.5 - 2.5 nm with a GaAs sublayer and 10% [P] within the QDash and WL covers a wavelength range of 1459-

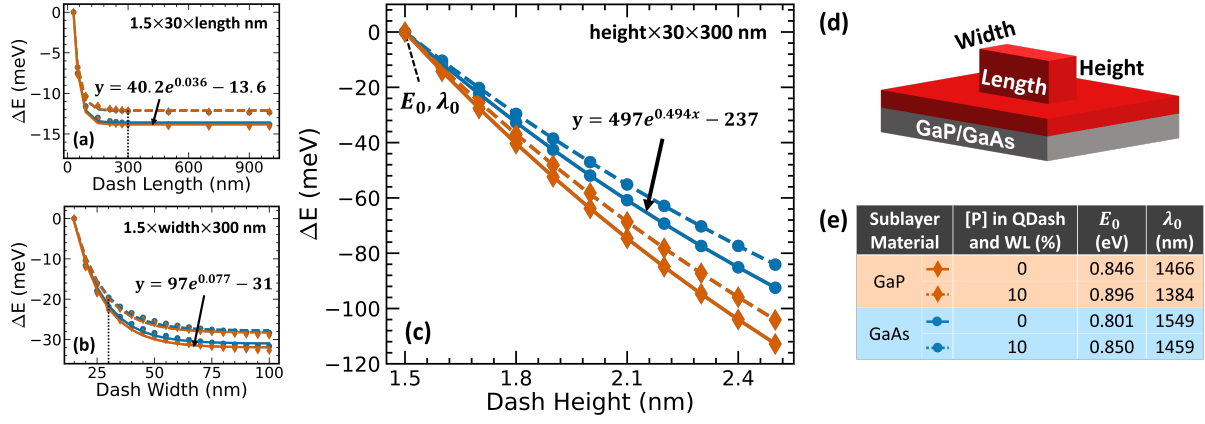


FIG. 4. Simulated change in emission energy with respect to initial wavelength λ_0 as a function of (a) QDash length, (b) QDash width, and (c) QDash height; (d) Diagram explaining QDash dimensions; (e) Simulation description and initial wavelengths for (c). Dashed lines in (a) and (b): default length and width chosen for all simulations. Outlined data points have emission wavelengths within experimental PL data range shown in Fig. 1(m).

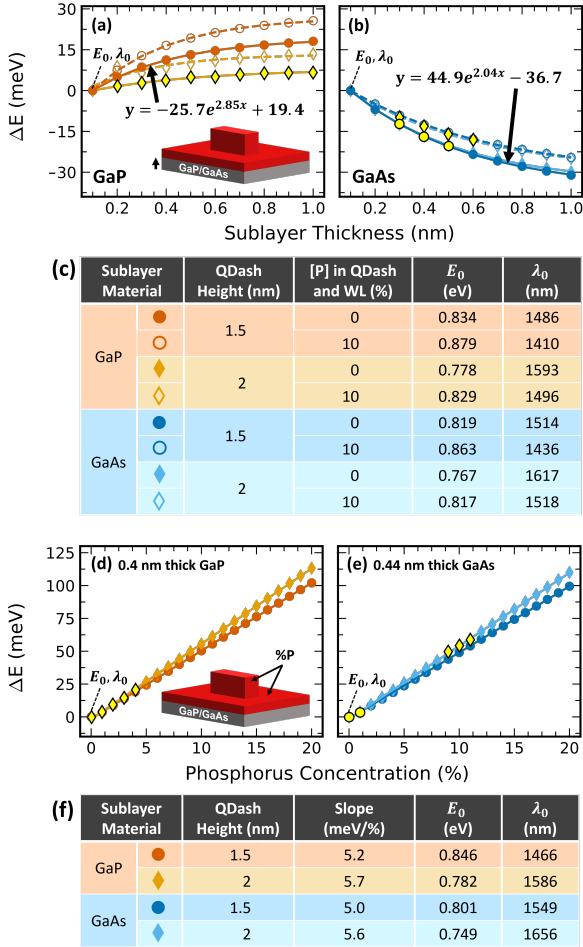


FIG. 5. Simulated change in emission energy as a function of (a) GaP and (b) GaAs sublayer thickness; (c) Simulation conditions and initial energies and wavelengths; (d,e) Change in emission energy as a function of QDash and WL [P]; (f) Simulation conditions and initial energies and wavelengths. Outlined data points have emission wavelengths within experimental PL data range shown in Fig. 1(m).

1620 nm, and is thus centered around 1550 nm, as shown in Fig. 4(c). Highlighted data points are simulation conditions that have transition wavelengths within the experimental PL range shown in Fig. 1(m). We see that despite only tuning for the default set of parameters, the PL and simulation wavelengths agree well for a variety of simulation conditions. We have thus demonstrated that from the conditions studied, a GaAs sublayer with a 0.5 nm WL, combined with either a 1.5 nm InAs QDash or 2.0 nm InAs_{0.90}P_{0.10} QDash, are well-suited for C-band emission.

Fig. 5(a) and (b) show the calculated change in the lowest QDash energy transition as a function of sublayer thickness. The lines, as in Fig. 4, are exponential fits, with conditions, initial energies, and wavelengths shown in Fig. 5(c). As we increase the thickness of the GaP sublayer in Fig. 5(a), the emission energy increases by almost 30 meV. This corresponds to a wavelength shift from 1486 nm to 1455 nm. The bandgap and offsets of GaP are larger than InGaAsP, thus increasing the thickness of the GaP sublayer provides higher confinement than an InGaAsP barrier, and we see a rise in the emission energy. Comparatively, as we increase the thickness of the GaAs sublayer in Fig. 5(b), the emission energy decreases since the band alignment of GaAs in the CB does not confine the mode as effectively as the InGaAsP barrier. In Fig. 3(c), we show that the first ten subbands for the 0.44 nm thick GaAs sublayer lie above the CB for GaAs. An increase in the thickness of this GaAs sublayer thus results in further mode spreading, and we see the energy levels shift towards the InAs band edges. Simulations run with a GaAs sublayer and 1.5 nm QDash and 2.0 nm QDash with 10% [P] have starting wavelengths of 1514 and 1518 nm, respectively. These are shown in Fig. 5(b), and reach emission wavelengths of 1550 nm for physically feasible thicknesses of between 0.4-0.6 nm. In contrast, simulated QDashes on GaP sublayers like those in Fig. 5(a) do not reach the target wavelength of 1550 nm. Fig. 5(d) and (e) show that increasing the [P] within the QDash and WL causes a decrease in wavelength by approximately 150-200 nm, or 100-115 meV, for 1.5 and 2 nm QDashes, respectively.

This is expected since the addition of phosphorus causes a decrease in compressive strain and band offset as seen in Fig. 3(c). The change in band offset is linear and thus the corresponding shift in energy levels is also linear, with slopes of the fits shown in 5(f). The trends appear almost identical regardless of sublayer type. QDashes with GaAs sublayers can be tuned to the desired wavelength of 1550 nm by incorporating phosphorus into the InAs layers during the growth process.

Single QDash energy level simulations have been performed for an InAs QDash with a GaP or GaAs sublayer, InP cap, and InGaAsP barriers. The physical dimensions are informed by AFM scans of uncapped InAs/InGaAsP/InP QDot and QDash arrays, and the model is tuned to match PL wavelengths of capped layers. Simulations confirm that the QDash height is the dominating physical dimension impacting the lowest energy transition, taken as the emission wavelength. Of the parameters investigated, the emission energy varies the most, by up to 120 meV, when QDash height and [P] vary within experimentally achievable ranges. This corresponds to a shift in emission wavelength of approximately 200 nm. The sublayer thickness and type is shown to play an active role in the energy levels in addition to controlling the morphology of nanoparticles. These simulations thus show that QDash height, using a GaAs sublayer, and modifying the [P] within the QDash and WL are the most practical parameters for tuning the emission energies of InAs/InGaAsP/InP QDashes for the C-band centre wavelength of 1550 nm.

SUPPLEMENTAL MATERIAL

Further information about the sample growth and layer structure can be found in the Supplementary Information file.

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Supplementary information for "Indium arsenide single quantum dash morphology and composition for wavelength tuning in quantum dash lasers"

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There are ten samples analyzed with atomic force microscopy (AFM) in this publication. All ten InAs/InGaAsP/InP nanoparticle samples are grown by chemical beam epitaxy on n-type (001) InP substrates using a Riber 32P reactor. The samples were grown at temperatures from 500 to 540°C, with trimethylindium and cracked arsine and phosphine precursors. The substrate temperature was monitored using an optical measurement of the substrate bandedge¹. All ten samples consist of five buried layers of InAs nanoparticles, an InP spacer, and five more layers of nanoparticles with the top layer left uncapped for AFM analysis. The growth process starts with an InP buffer deposition, onto which the InGaAsP quaternary is grown with a room temperature PL peak at 1.15 μm . A 0.4 nm (GaP) or 0.44 nm (GaAs) thick sublayer is deposited, followed by InAs with a growth interruption to allow nanoparticle formation via the Stranski-Krastanow mode. The nanoparticles are capped with InP in a double-step deposition procedure² with a growth interruption to homogenize the QDot and QDash heights³. During this process, there is As/P intermixing between the InP and InAs layers. While the growth process has been developed to grow arsenic-rich nanoparticles for maximum strain, full suppression of the As/P intermixing

has not been experimentally confirmed. The period of the nanoparticle stacks from InGaAsP barrier to barrier is 11 nm and 15.5 nm for GaAs and GaP sublayers, respectively. The nominal InP thickness is 1.4 nm for GaAs sublayers and 2 nm for GaP, where the InP will fill between and on top of the nanoparticles. Information about similar growths can be found in publications by Poole et al.²⁻⁵.

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Chapter 6: Effect of Wetting Layer on Emission Energy and Overlap Integrals

6.1 Effect of Wetting Layer on Emission Energies

In the previous chapter, the effect of phosphorus concentration and sublayer type were discussed with a constant WL thickness of 0.5 nm. When phosphorus concentration was varied it was in both the wetting layer and the QDash itself. In this section we will consider the effect of the wetting layer on emission wavelength in more detail.

There has been substantial experimental research about the effect of sublayers, growth parameters, and growth processes on InAs/InP nanoparticle formation. With respect to the InAs WL formed during the self-assembly process, there has been much deliberation about its existence post-InP capping process. It has been shown in previous publications that the As/P exchange when growing these InAs/InP self-assembled QDots and QDashes can be suppressed using GaAs or InGaAs sublayers [34], [35]. Increasing the thickness of the GaAs sublayer from 0 to 2.5 monolayers has been shown to reduce the overall size of the nanoparticles and both the PL wavelength and line width. This is a consequence of the reduced As/P exchange, which will redshift the nanoparticle PL emission [35].

It has also been shown that as the InAs WL forms during the self-assembly it can prevent further As/P exchange between the previous epilayers and the InAs nanoparticles. Indeed, there has been contradicting evidence both that the nanoparticles themselves will not change composition during the self-assembly process itself and will remain a pure InAs binary [36], or that InAsP nanoparticles will form [37]. It has also been demonstrated that an InAsP alloy will be formed at the interface of compounds containing P and As - the WL underneath the nanoparticles - due to this element intermixing [36], [38]. There is yet more evidence that the WL will see a large amount of intermixing, as [39] cites only 29% As within an InAsP WL for QDots capped with InP. The amount of intermixing depends on growth conditions, notably the growth interruption times between the deposition of the InP cap. The change in composition also yields a modification in the strain. Since these nanoparticles are formed due to self-assembly, the strain profile of the QDash is anisotropic across the surface of the QDash, within it, and within the WL. The resulting strain profile from experimental data can be used as an indication of the composition across a cross-section of the nanoparticle.

With these concepts in mind, in this chapter we explore the effect of varying just the WL com-

position on the predicted emission wavelength of single QDashes. While an anisotropic strain profile has yet to be initialized in these single QDash simulations in Crosslight, the bulk strain modification as a result of changing the layer composition can be an adequate representation of how these parameters will affect the predicted energy levels and therefore emission energies.

As in Chapter 5, the QDash is maintained at $30 \text{ nm} \times 300 \text{ nm}$ lateral dimensions while varying the height of the QDash, removing the WL, and modifying the phosphorus concentration. We note that the QDash height is re-defined in this chapter as the height from the top of the sublayer to the top of the QDash, whereas in the previous chapter it was defined as the top of the WL to the top of the QDash. A visual representation of the way the QDash height is defined for this chapter is shown in the right-hand figures in Fig. 6.1.

6.1.1 QDash Height and the Wetting Layer

Before we consider the effect of phosphorus concentration, we first investigate the difference in transition energy with and without the 0.5 nm WL which is shown in Fig. 6.1. The y-axis is defined as the difference of the energy at QDash height x and the energy of the first data point (2 nm QDash height): $\Delta E = E_{\text{height}x} - E_{\text{height}2\text{nm}}$.

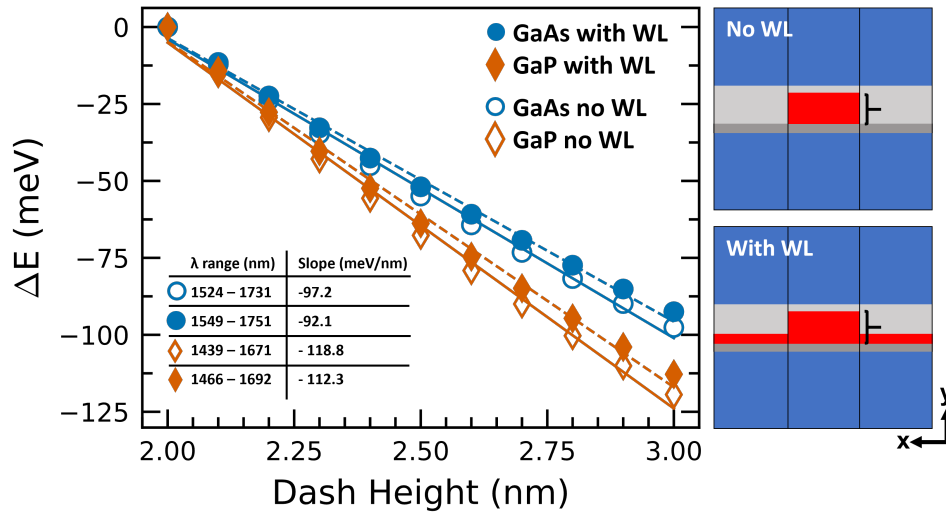


Figure 6.1: Effect of varying QDash height on the emission energy for both with and without WL. The effect is similar for both GaP and GaAs sublayers. The definition of QDash height is modified to account for comparing no WL to WL conditions as shown on the right.

As visible from the inset table in the figure, we can see that the WL contributes an increase in

the emission wavelength of approximately 25 nm. It also reduces the slope of the linear fits by ~ 5 meV/nm for the GaAs sublayer, and almost 7 meV/nm for the GaP sublayer. Overall, this means that without the WL, the rate of change of ΔE with the QDash height is higher. The WL decreases the transition energy, however the trend remains the same regardless of its presence. Since the presence of a WL for the InAs/InP material system is under debate, this solidifies that it has negligible effect on the behaviour of the first transition energy. However, while the WL may not impact the first transition energy it still significantly affects carrier dynamics and optical properties of QDash layers [19], [23], [40].

6.1.2 Phosphorus Concentration and the Wetting Layer

Three separate datasets are investigated in this section, and shown in Fig. 6.2: (1) the first is the same as in Chapter 5.2 and is used as a reference, where the phosphorus concentration in both the QDash and the WL is varied from 0-20%. In (2), the phosphorus concentration is changed solely in the 0.5 nm WL, while the QDash composition remains purely InAs. In the third dataset (3), everything but the portion of the WL under the QDash is replaced with InP. Essentially, the WL is removed and a 0.5 nm thick section underneath the QDash varies from 0-20% phosphorus.

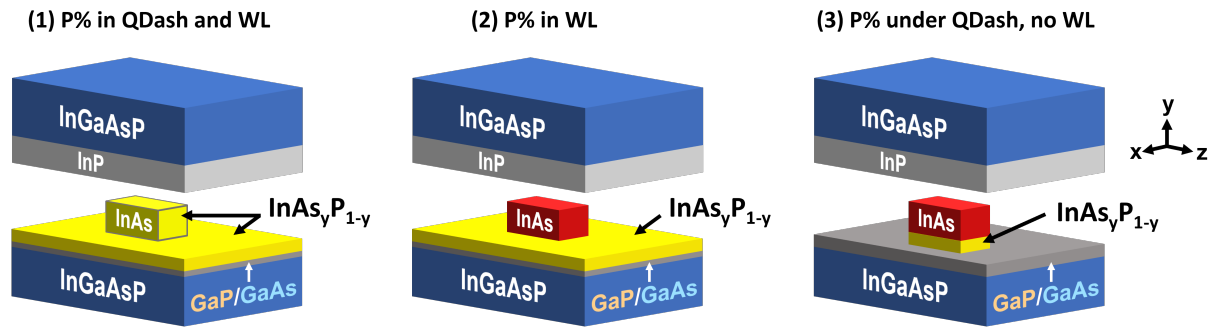


Figure 6.2: Three phosphorus concentration conditions: (1) P% in both the QDash and WL, (2) P% in just the WL, and (3) P% in equivalent WL height component of QDash ("under QDash condition") with no WL.

The Crosslight simulations take into account this change in composition within the bandgap calculation and therefore the uniform strain percentage in the changing layer. The bandgap diagrams generated by Crosslight PICS3D are shown in Fig. 6.3. As phosphorus concentration increases, the bandgap of the relevant layers increases due to a change in band offset for both the VB and the CB. The default band offsets provided by Crosslight's macro library are used.

As described in Chapter 5.2 Fig. 3, the VB offset changes at a faster rate than the CB offset for increasing phosphorus concentration. For condition (1), the phosphorus concentration changes throughout the entire QDash and WL layers; the bandgap is modified uniformly across this region as shown in the left bandgap in Fig. 6.3. For condition (2), the bandgap of the WL changes by the same amount, but the QDash bandgap remains the same. Condition (3) is similar to condition (2), except the band structure only changes in the range $30 < x < 60$ nm, as the WL is removed and only the region underneath the QDash changes in composition.

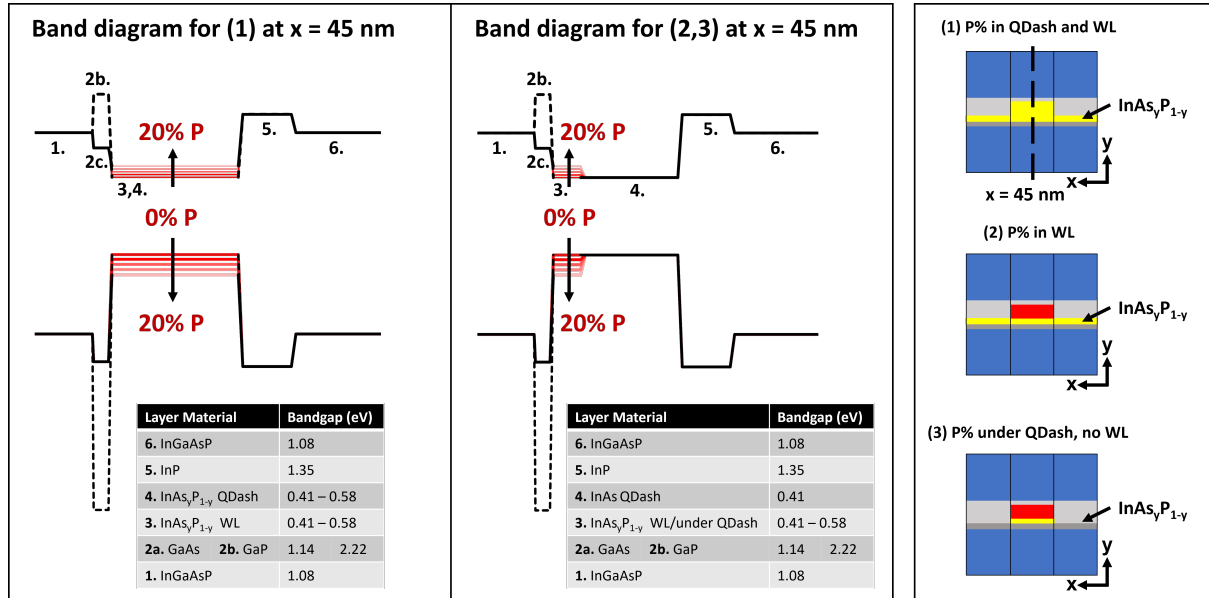


Figure 6.3: Bandgap diagram through QDash ($x = 45$ nm) for three phosphorus concentration conditions: (1) P% in both the QDash and WL, (2) P% in just the WL, and (3) P% in equivalent WL height component of QDash ("under QDash condition") with no WL.

Fig. 6.4 shows the relationship between the transition energy and the phosphorus concentration within the WL due to the band structure changes. Case (1), where phosphorus concentration changes in both the QDash and WL, is discussed in detail in section 5.2 of this thesis. Thus, this figure looks at cases (2) and (3), where the phosphorus concentration changes in just the WL or the portion underneath the QDash, respectively. We immediately see that as the WL composition changes from pure InAs, just like the QDash, to 1% phosphorus, there is a drastic change in the emission energy. This is due to the fact that the effective QDash height in the centre decreases by 0.5 nm as soon as the WL composition changes from that of the QDash. As the concentration then increases from 1% to 20%, we see similar trends for sublayer type, QDash height, and for with or without a WL. Interestingly, for the phosphorus composition changing just under the QDash with no WL, the slope of the change in emission energy is larger,

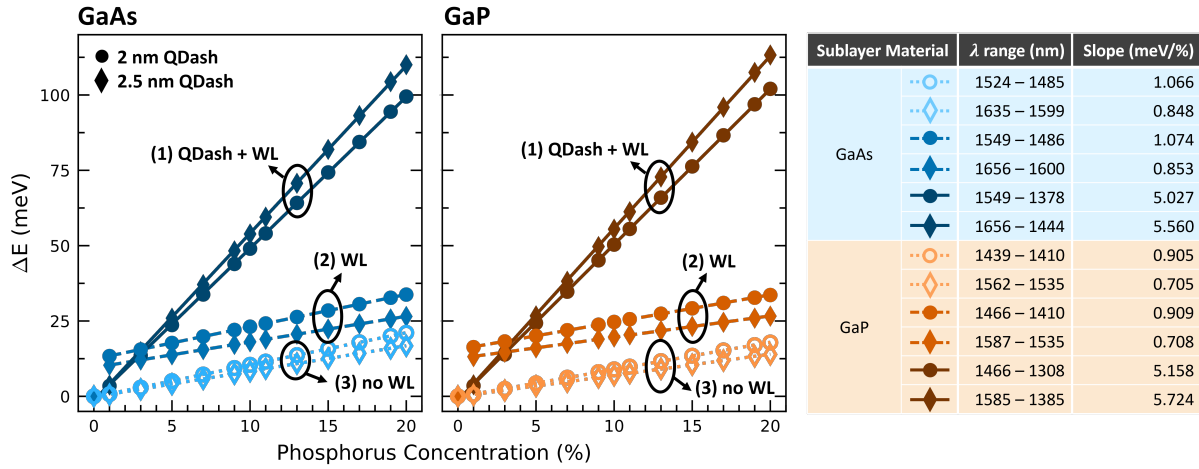


Figure 6.4: Effect of varying phosphorus concentration for conditions (1) QDash + WL, (2) just in the WL ("WL") and (3) in the 0.5 nm portion just under the QDash ("no WL"). For both GaAs (left) and GaP (right) sublayers.

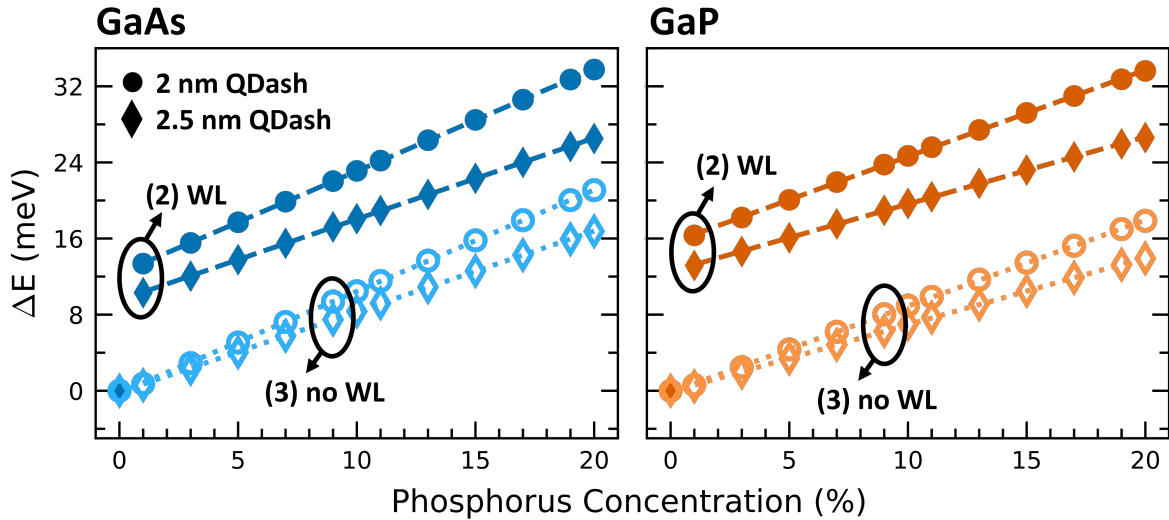


Figure 6.5: Effect of varying phosphorus concentration for conditions (2) just in the WL ("with WL") and (3) in the 0.5 nm portion just under the QDash ("no WL"). For both GaAs (left) and GaP (right) sublayers.

implying that the lack of WL increases the sensitivity of the change in emission energy with respect to phosphorus concentration. There is a slightly higher rate of change for conditions (2) and (3) for the 2 nm height QDash than the 2.5 nm in both sublayer types. This occurs because the region where the phosphorus concentration is changing is a larger proportion of the entire InAsP height than for the taller QDash. When compared to condition (1), we see that this trend

reverses. For phosphorus concentrations changing in both the QDash and WL, it follows that the taller the QDash the higher the rate of change in emission energy will be as the composition of both the WL and QDash remains the same. Fig. 6.5 shows the change in emission energy as a function of phosphorus concentration for conditions (2) and (3) in more detail.

6.2 Overlap Integrals and Mode Confinement

As described in Chapter 2.3.2, the overlap integral can be calculated using Crosslight as a measure of mode confinement within the QDash. The overlap integral, depicted as a value from 0-1, is a quantitative measure of the overlap between the hole wavefunction in the VB subband and the electron wavefunction in the CB subband. The closer the value is to 1, the greater the spatial overlap between the two wavefunctions and the higher the probability of the transition. In this section we investigate how the overlap integral changes as a function of parameters discussed in prior sections: the QDash dimensions: height, width, and length; GaAs and GaP sublayer thicknesses; and our three phosphorus concentration conditions (1) QDash + WL, (2) WL, and (3) under QDash, no WL.

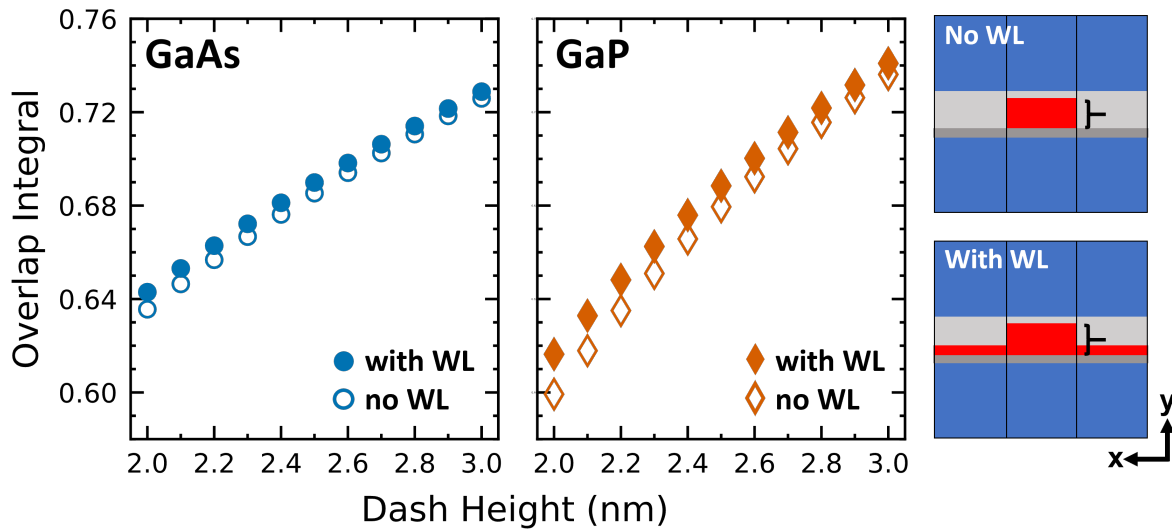


Figure 6.6: Effect of QDash height on overlap integral for both GaAs and GaP sublayers. Lateral dimensions of QDash are 30 nm×300 nm.

Fig. 6.6 shows the overlap integral as a function of QDash height for both GaAs and GaP sublayers with and without a WL. We see that the overlap integral increases as the QDash height increases, which we expect as a taller nanoparticle will increase confinement of the wavefunc-

tion. The presence of a 0.5 nm pure InAs WL underneath the QDash, which is included in the total QDash height, has negligible effects on the overlap integral. As the QDash height increases, the discrepancy between the overlap integrals calculated for QDashes with and without the WL is reduced for both sublayer types. GaAs, despite providing shorter valence band offsets as shown in Fig. 6.3 and therefore lower confinement, still produces comparable overlap integrals to GaP sublayers. It should be noted that this could partially be a consequence of the 0.44 nm thick GaAs sublayer, while the GaP sublayer is slightly thinner at 0.4 nm. This could also explain the smaller overall change in overlap integral as a function of QDash height for a GaAs sublayer over a GaP sublayer. From a transition probability perspective, the presence of a WL is inconsequential to whether the transition will occur.

In Fig. 6.7, the overlap integrals as a function of QDash width and length follow the same trend as their change in emission energy counterparts shown in Chapter 5.2. The transitions become more and more likely as the lateral dimensions of the QDash are increased. For the QDash length in particular, it becomes invariant at around 175 nm when the other QDash dimensions are set to 30 nm $\times$ 300 nm.

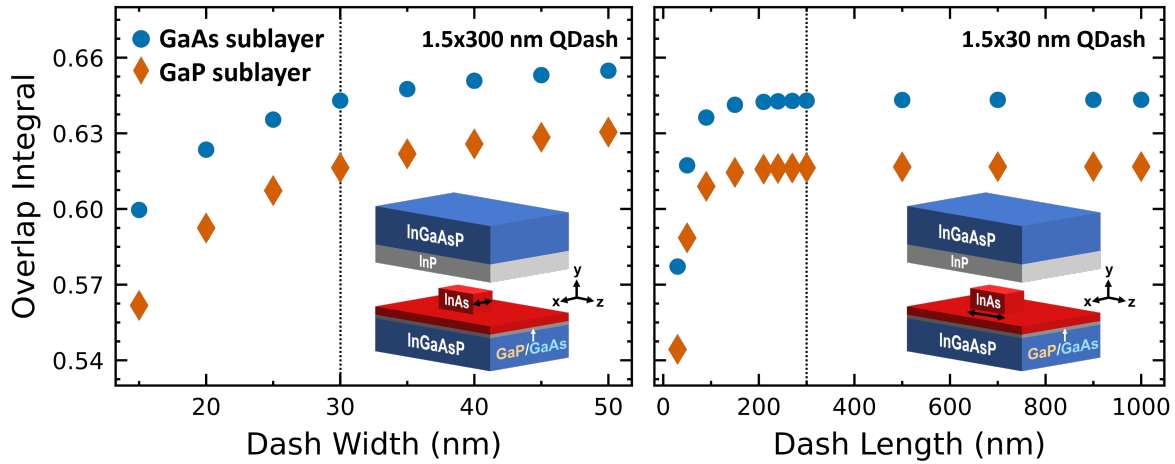


Figure 6.7: Effect of QDash width (left) and length (right) on overlap integral for both GaAs and GaP sublayers.

The thickness of the sublayer for all previous simulations was set to 0.4 nm for GaP and 0.44 nm for GaAs in compliance with nanoparticle growths from National Research Council Canada. In Fig. 6.8 we now explore what happens to the overlap integral when the thickness of both GaP and GaAs sublayers are varied. Conversely to the QDash dimensions, the overlap integral as a function of sublayer thickness does not follow the same trend as the change in emission energy shown in Chapter 5.2. As the sublayer thickness is increased from 0.1 nm, the overlap integral

decreases for both sublayer types. At approximately 0.6 nm, there is an inflection point and the overlap integral for the GaP sublayer begins to increase.

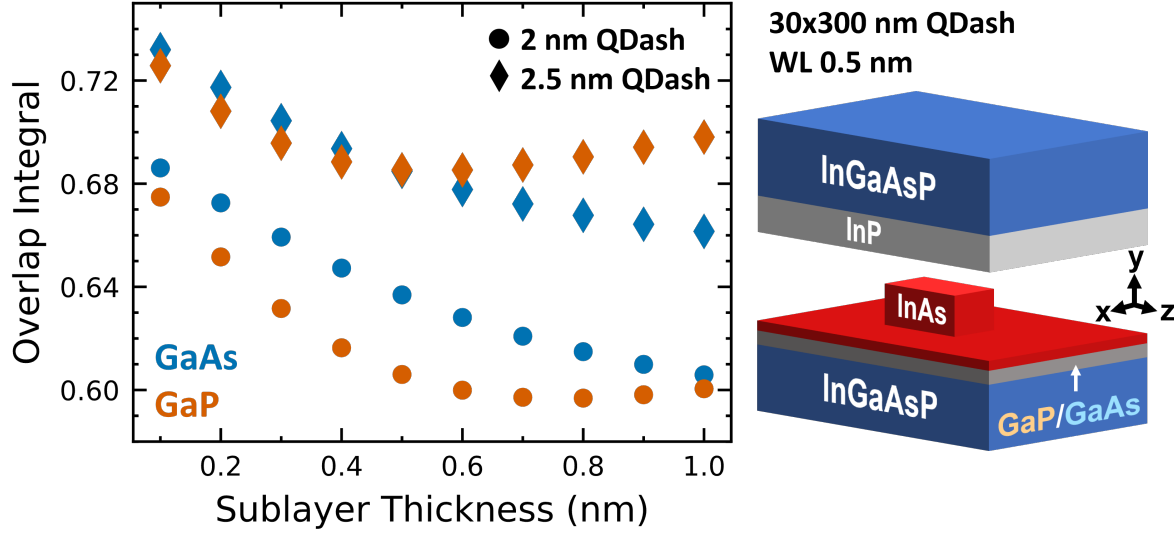


Figure 6.8: Effect of sublayer thickness on overlap integral for QDash heights of 2 and 2.5 nm and both sublayer types.

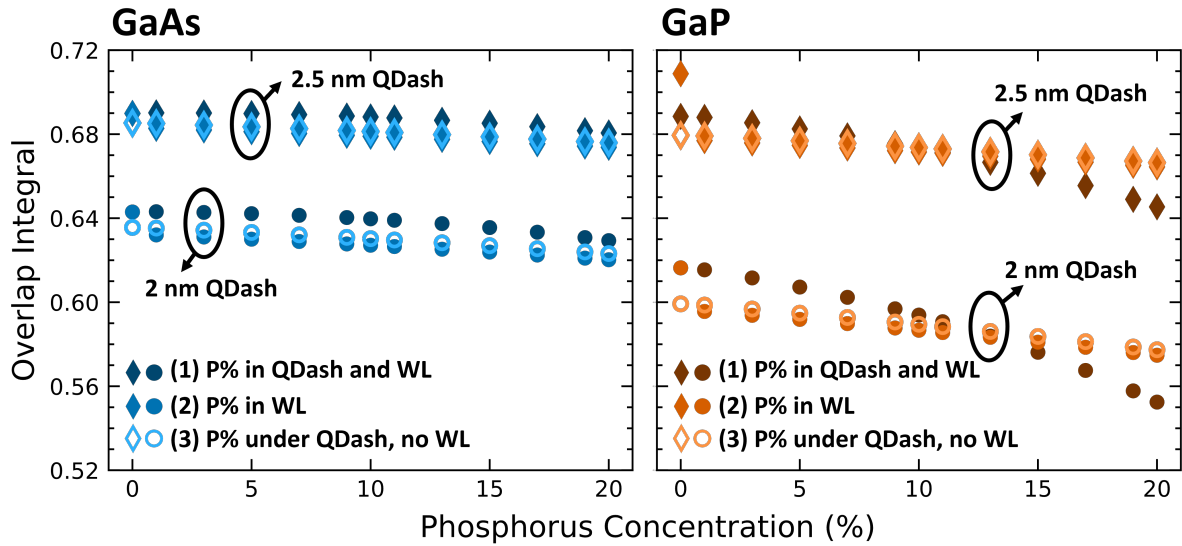


Figure 6.9: Effect of phosphorus concentration on overlap integral for QDash heights of 2 and 2.5 nm and both sublayer types.

Finally, we summarize the effect on overlap integral due to increasing phosphorus concentration in our three conditions, shown in Fig. 6.9. As expected, the QDash height increases the over-

lap integral, however there is negligible difference between all three cases for GaAs sublayers. Simulations with GaP sublayers for condition (1) have overlap integrals that vary by approximately 7%, as compared to approximately 3% for GaAs sublayers. This can be explained by the fact that the band offset between the GaP sublayer and the InAsP WL and QDash layers decreases in both the VB and CB, therefore reducing confinement and allowing the wavefunctions to spread further as phosphorus content increases. This is less pronounced for conditions (2) and (3) for the same reasons as described for the change in emission energy. Also as expected, for condition (2) at 0% phosphorus, we see a spike in the overlap integral. This is because the QDash and WL have the same composition at this point, after which the effective QDash height drastically decreases once the WL has increasing phosphorus concentration. We see the same effect for the change in emission energy. It is more prominent for GaP, since there is greater confinement with this sublayer type.

Chapter 7: Conclusions

7.1 Further Research

The following section presents several recommendations for extensions to this project, for both experimental work and simulations.

For experimental work, we recommend further exploration of the capped nanoparticles to ascertain the compositional and morphological changes. While scanning electron microscopy (SEM) and transmission electron microscopy (TEM) are used for imaging QDots and QDashes, they do not allow for compositional resolution. Cross-sectional scanning tunneling spectroscopy (STS) has shown promise for analyzing buried quantum dashes for compositional information [3], [41].

As continuation of the simulations performed, integrating a variable strain and composition profile within the QDashes would better represent experimental findings. Crosslight PICS3D does allow for custom strain and composition profiles within the layer structure, and thus we recommend continuing to use this software. However, exploration of $\mathbf{k} \cdot \mathbf{p}$ simulators for further simulations would allow for more complicated strain effects and valence band intermixing to be modelled. In addition, Crosslight's box_single model was primarily developed for QDots, and as such uses a zero-dimensional density of states. Modification of this to a quasi-one-dimensional density of states is recommended for a closer experimental match.

All of the simulations in this thesis were performed at a default 300 K; investigating how the bandgap and energy level spacing changes as a function of temperature would be valuable for laser applications. In addition, the strain profile within QDashes and QDash arrays not only affects the morphology of the single nanoparticles, but can also induce vertical alignment when multiple stacks are grown [19], [23], [29]. As such, we recommend performing simulations of vertically stacked QDashes to investigate the coupling of nanoparticles.

7.2 Conclusion

This thesis is an experimental and theoretical investigation of the effect of QDash morphology and composition on energy level spacing and emission energy. QDash arrays are promising laser gain media due to their unique density of states and discretization of energy levels within the

nanoparticles. Our study began with an experimental analysis of uncapped InAs/InGaAsP/InP QDashes under varying growth conditions. In section 4.2, a straightforward method was developed and used to characterize uncapped QDash heights using AFM. We determined QDash heights on the order of 1.5 to 2.5 nm, measured via our three Gaussian fit approach, and discussed the effect of the InP capping process on controlling QDash height. The average nanoparticle widths and surface densities were also summarized. We also established that QDash heights from 1.5 to 2.0 nm were practical for QDash simulations.

The next two chapters presented simulations of single QDashes performed using Crosslight PICS3D. These simulations were tuned to experimental parameters determined in preceding sections and PL data provided from National Research Council Canada. In Chapter 5, we summarized the effect of QDash dimensions, QDash and WL composition, and sublayer thickness on the energy level spacing within the single QDash. In Chapter 6, we present further investigation of the presence of an InAs WL and its effect on emission energy. We also show emission energies for three datasets of phosphorus concentration: increasing phosphorus content within (1) the QDash and WL, (2) the WL, and (3) under the QDash with no WL. We discussed the relationship between QDash dimensions, composition, and sublayer type on the overlap integral, an indicator of transition probability.

Further exploration of the nature of these QDashes is integral to the creation of increasingly efficient, cost-effective, and robust QDashLs. This thesis recommends further experimental analysis of QDashes via TEM, SEM, or X-STM/STS. The single QDash simulations presented here are a starting point that can build towards models with vertically coupled QDashes and a more complex strain and composition profile.

Chapter 8: Appendix

8.1 Processed AFM images

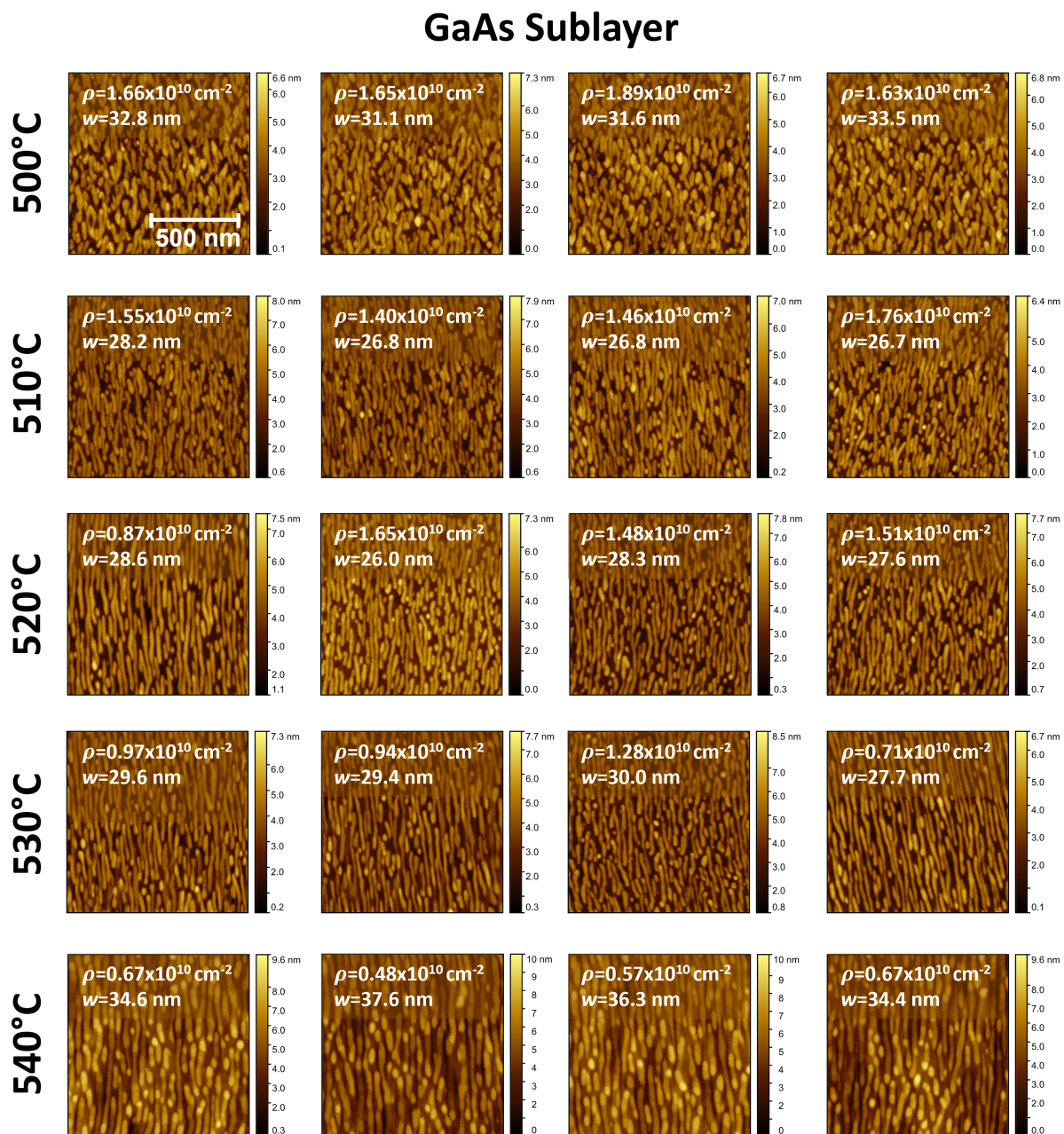


Figure 8.1: Overview of GaAs sublayer $1 \mu\text{m}^2$ AFM images.

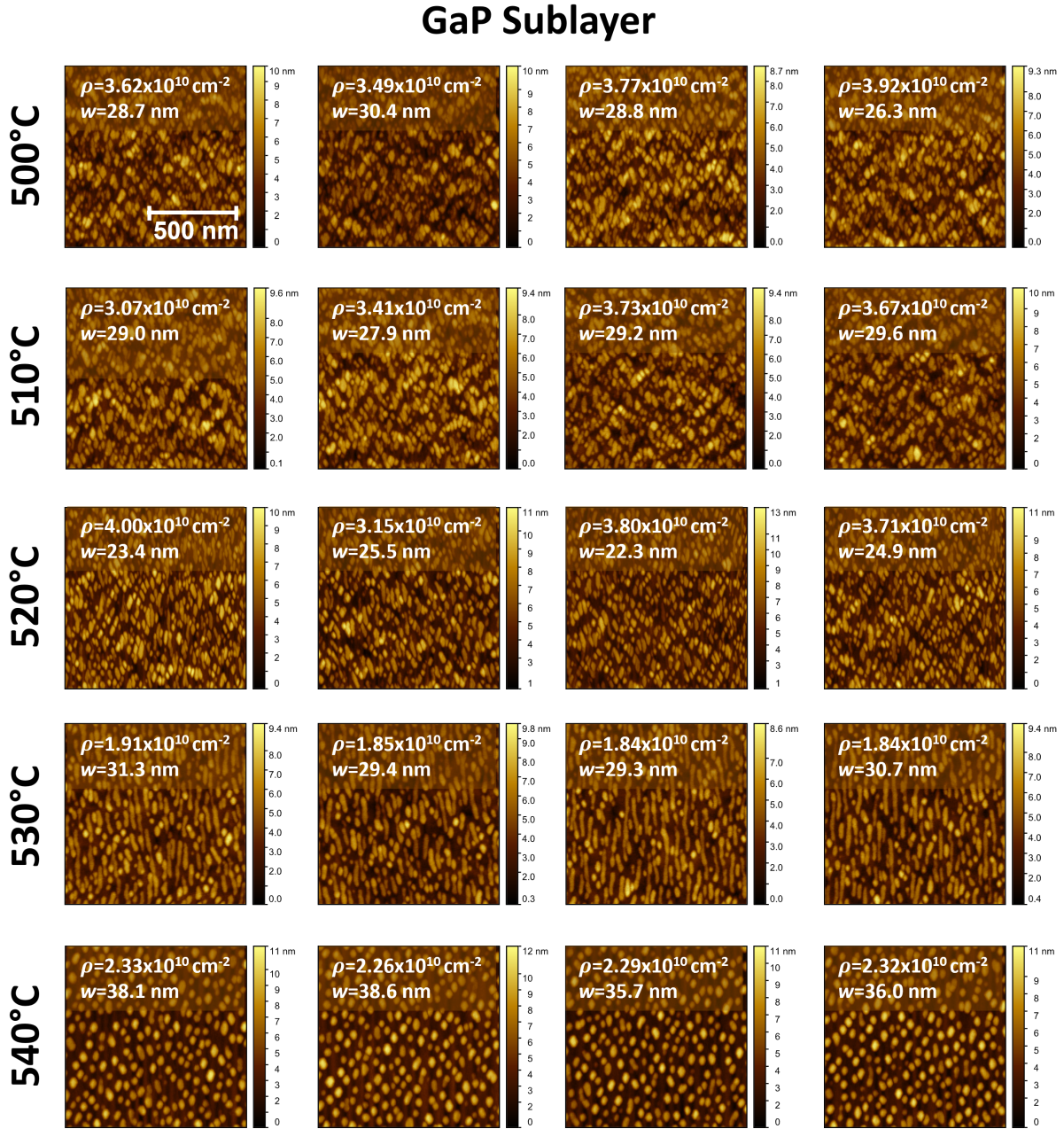


Figure 8.2: Overview of GaP sublayer $1 \mu\text{m}^2$ AFM images.

8.2 AFM Data Processing

8.2.1 AFM Height Distributions of $1\ \mu\text{m}^2$ AFM images

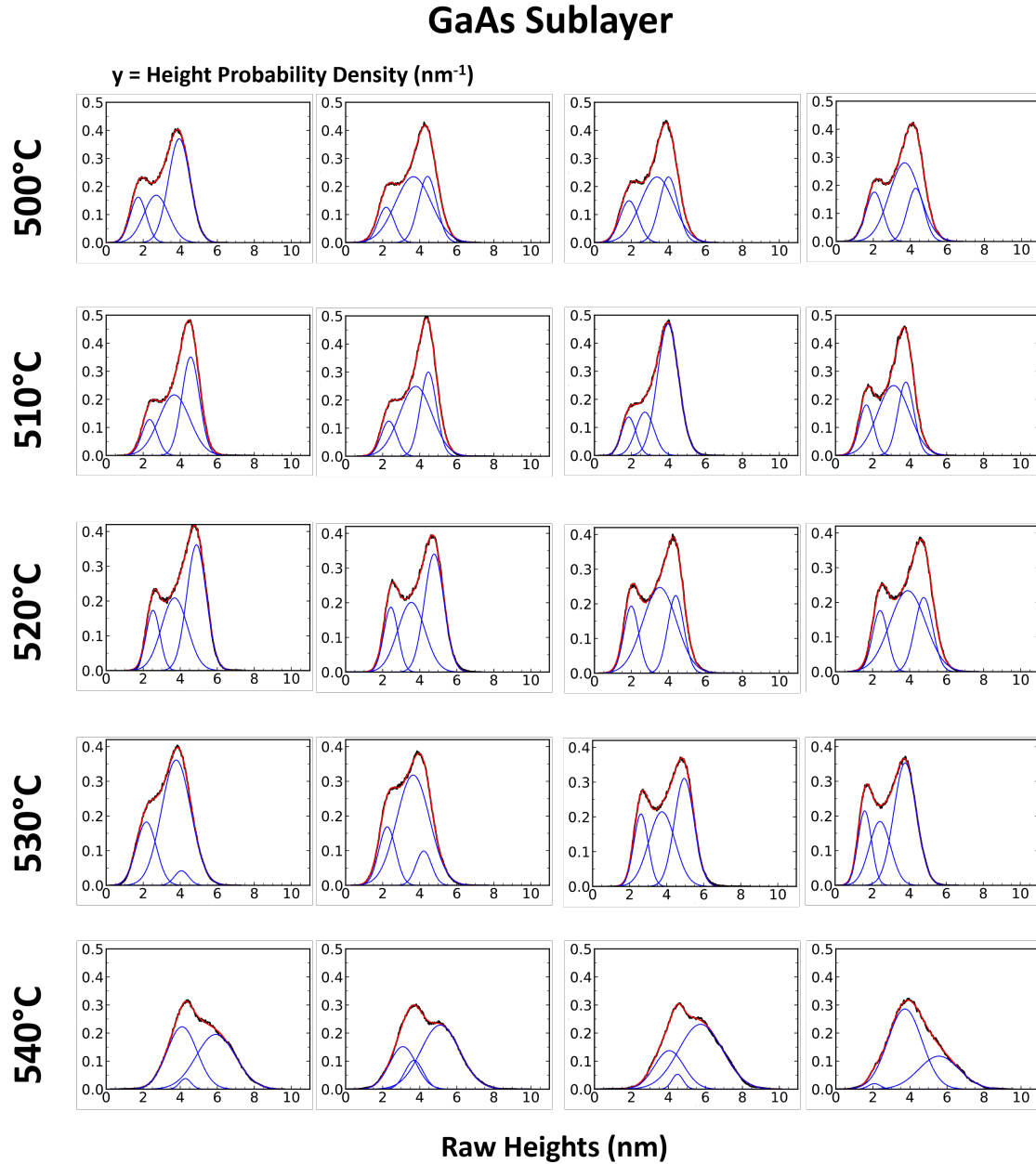


Figure 8.3: Overview of height distribution plots for GaAs sublayer $1\ \mu\text{m}^2$ AFM images.

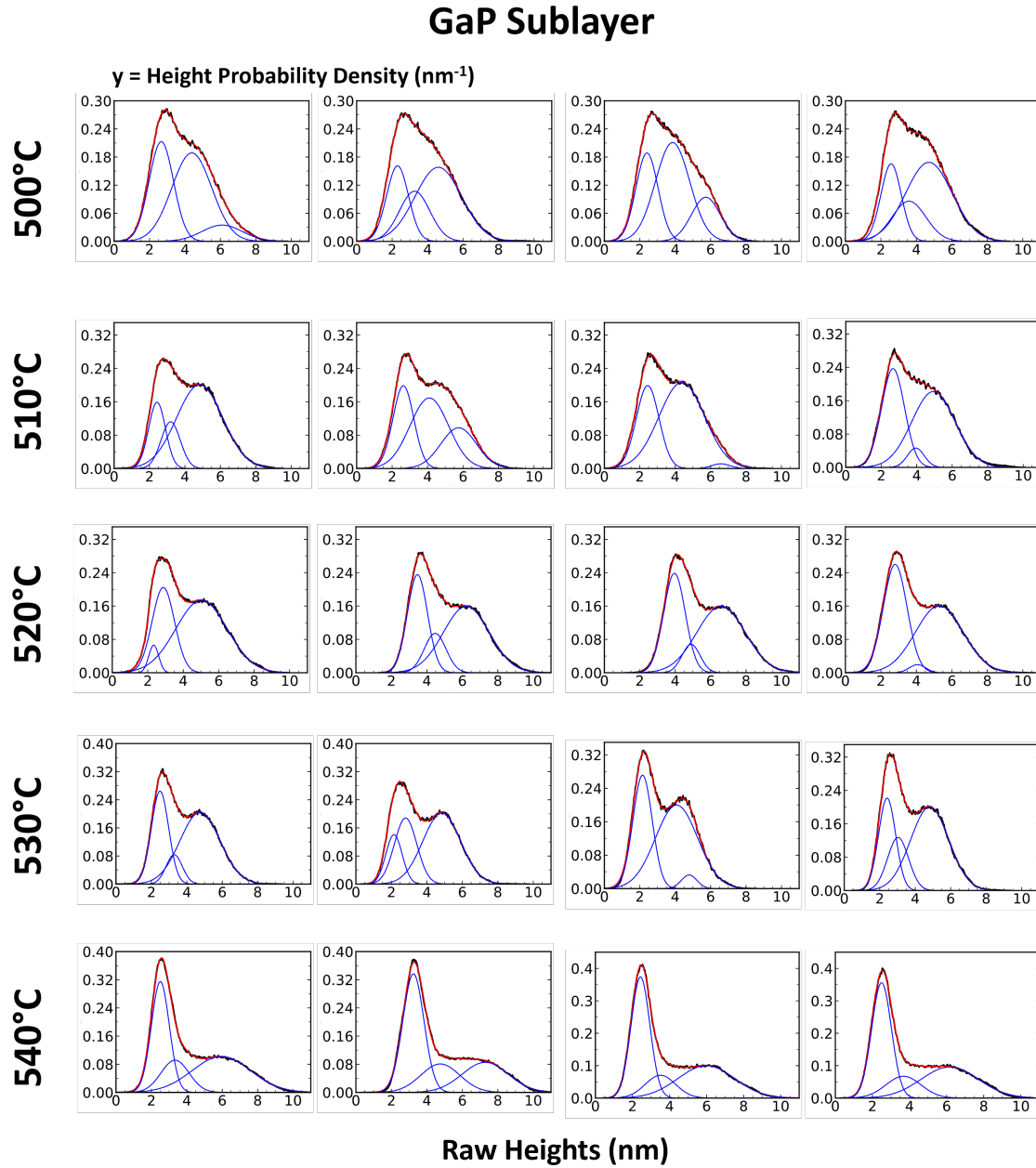


Figure 8.4: Overview of height distribution plots for GaP sublayer 1 μm^2 AFM images.

8.3 Crosslight Simulation Code

8.3.1 Layer Files

The macro setup format for these files follows the InGaAsP quaternary installed in Crosslight's macro database. The variables represent: $\text{In}_{(1-x)}\text{Ga}_x\text{As}_y\text{P}_{(1-y)}$. Thus binaries are approximated

by associating the relevant parameter(s) with $x = 0.0001$ instead of $x = 0$. As a reminder, the nomenclature for denoting boxes and columns in the PICS3D LayerBuilder is described in Fig. 3.4. The following files are copied verbatim from Crosslight. All the files shown here are for the 1.5nm tall QDash with a GaAs sublayer case.

Box1 .layer File for 1.5nm QDash with GaAs sublayer

```
begin_layer
internal_xpoint xp_size=1e-4
$
$ when we have more than one columns of complex structure, indep_xmqw
$ is needed.
column column_num=1 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=2 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=3 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
$
$Lower 1.15Q layer, mater_lib macro
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=0.9
$
$GaAs/GaP layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer d=0.00044 n=5 r=1.
$
$InAs wetting layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
```

```

model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$
$InP surrounding InAs dot, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0015 n=16 r=1.
$
$InP capping layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$
$Upper 1.15Q layer, mater_lib macro no model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&

```

```

var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=1.1
$
end_layer

```

Box2 .layer File for 1.5nm QDash with GaAs sublayer

```

begin_layer
$
internal_xpoint xp_size=1e-4
previous_layer file=box1.layer
$ when we have more than one columns of complex structure, indep_xmqw
$ is needed.
column column_num=1 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=2 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=3 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
$
$Lower 1.15Q layer, mater_lib macro
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=0.9
$
$GaAs/GaP layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer d=0.00044 n=5 r=1.
$
$InAs wetting layer, mater_lib macro with model=quantum_well

```

```

layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$
$InP surrounding InAs dot, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0015 n=16 r=1.
$
$InP capping layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well

```

```

layer d=0.0005 n=6 r=1.
$
$Upper 1.15Q layer, mater_lib macro no model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=1.1
$
end_layer

```

Box3 .layer File for 1.5nm QDash with GaAs sublayer

```

begin_layer
internal_xpoint xp_size=1e-4
$
previous_layer file=box2.layer
$ when we have more than one columns of complex structure, indep_xmqw
$ is needed.
column column_num=1 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=2 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
column column_num=3 w=0.030 mesh_num=16 r=1. indep_xmqw=yes
$
$Lower 1.15Q layer, mater_lib macro
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=0.9
$
$GaAs/GaP layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.9999 var_symbol2=y var2=0.9999 &&

```

```

model=quantum_well
layer d=0.00044 n=5 r=1.
$
$InAs wetting layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.9999 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$
$InP surrounding InAs dot, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0015 n=16 r=1.
$
$InP capping layer, mater_lib macro with model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&

```

```

model=quantum_well
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.0001 var_symbol2=y var2=0.0001 &&
model=quantum_well
layer d=0.0005 n=6 r=1.
$Upper 1.15Q layer, mater_lib macro no model=quantum_well
layer_mater mater_lib=InGaAsP column_num=1 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=2 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer_mater mater_lib=InGaAsP column_num=3 &&
var_symbol1=x var1=0.185 var_symbol2=y var2=0.405
layer d=0.05 n=10 r=1.1
$
end_layer

```

8.3.2 Solution File box.sol for 1.5nm QDash

```

$*****
begin
3d_solution_method 3d_flow=yes
z_structure uniform_zseg_from=0 uniform_zseg_to=0.300 zseg_num=1 zplanes=20
z_structure uniform_zseg_from=0.300 uniform_zseg_to=0.600 zseg_num=2 zplanes=20
z_structure uniform_zseg_from=0.600 uniform_zseg_to=0.900 zseg_num=3 zplanes=20
load_mesh mesh_inf=box1.msh zseg_num=1
load_mesh mesh_inf=box2.msh zseg_num=2
load_mesh mesh_inf=box3.msh zseg_num=3
output sol_outf=box1.out
begin_zmater zseg_num=1
include file=box1.mater
include file=box1.doping
end_zmater
begin_zmater zseg_num=2
include file=box2.mater
include file=box2.doping
end_zmater
begin_zmater zseg_num=3
include file=box3.mater
include file=box3.doping
end_zmater
wave_boundary point_ll=(0. 0.) point_ur=(0.090 0.10338)
init_wave init_wavel=1.50

```

```

multimode mode_num=10 boundary_type1=(1 1 1 1)
sparse_eigen_solver use_mf=yes
direct_eigen
solve_lateral_wave quantum_wave=yes cond_valley=1 val_valley=1 &&
  export_data=box.qdd
solve_lateral_wave quantum_wave=yes cond_valley=1 val_valley=2
solve_lateral_wave quantum_wave=yes cond_valley=2 val_valley=1
$
end

```

8.3.3 Output File box.qdd and Processing

The most crucial output file for these simulations is the box.qdd file. This contains all the sub-band energies and overlap integrals for the first ten subbands within the HH, LH, Γ valley CB, and L valley CB. The variables "jc" and "jv" are used to represent CB and VB. For CB: indices 1 and 2 represent the Γ and L valleys, respectively. For VB: 1 and 2 represent HH and LH, respectively.

The box.qdd Output File

```

=====Start QM Wave Solver==jc jv=>          1          1
          0 Number of 2nd-set states to be searched
Overlaps between cond. and val. subbands
          10          10
1      1  0.671589
1      2  0.278319E-09
1      3  0.406331E-04
1      4  0.403535E-10
1      5  0.116210E-04
1      6  0.139926E-10
1      7  0.501917E-05
1      8  0.603838E-11
1      9  0.248012E-05
1     10  0.280855E-11
2      1  0.324230E-09
2      2  0.670530
2      3  0.891203E-09
2      4  0.125257E-03
2      5  0.124886E-09
2      6  0.361115E-04

```


2	7	0.435574E-10
2	8	0.156936E-04
2	9	0.188121E-10
2	10	0.767732E-05
3	1	0.467354E-04
3	2	0.113816E-08
3	3	0.668776
3	4	0.182918E-08
3	5	0.241748E-03
3	6	0.242606E-09
3	7	0.678364E-04
3	8	0.829801E-10
3	9	0.289155E-04
3	10	0.352645E-10
4	1	0.628682E-10
4	2	0.153109E-03
4	3	0.255713E-08
4	4	0.666341
4	5	0.314698E-08
4	6	0.386679E-03
4	7	0.397947E-09
4	8	0.104662E-03
4	9	0.132544E-09
4	10	0.431843E-04
5	1	0.157497E-04
5	2	0.226941E-09
5	3	0.314542E-03
5	4	0.479981E-08
5	5	0.663249
5	6	0.493798E-08
5	7	0.557140E-03
5	8	0.600949E-09
5	9	0.144989E-03
5	10	0.194357E-09
6	1	0.354487E-10
6	2	0.536401E-04
6	3	0.508529E-09
6	4	0.535754E-03
6	5	0.818470E-08
6	6	0.659535
6	7	0.733702E-08
6	8	0.749369E-03
6	9	0.865486E-09

6	10	0.187011E-03
7	1	0.875214E-05
7	2	0.137917E-09
7	3	0.110477E-03
7	4	0.949562E-09
7	5	0.821944E-03
7	6	0.131636E-07
7	7	0.655250
7	8	0.105241E-07
7	9	0.957754E-03
7	10	0.120778E-08
8	1	0.288298E-10
8	2	0.311194E-04
8	3	0.321775E-09
8	4	0.186761E-03
8	5	0.161100E-08
8	6	0.117661E-02
8	7	0.203648E-07
8	8	0.650465
8	9	0.147253E-07
8	10	0.117368E-02
9	1	0.603136E-05
9	2	0.119180E-09
9	3	0.651321E-04
9	4	0.616577E-09
9	5	0.283108E-03
9	6	0.257735E-08
9	7	0.159894E-02
9	8	0.306421E-07
9	9	0.645287
9	10	0.202094E-07
10	1	0.287325E-10
10	2	0.220228E-04
10	3	0.289135E-09
10	4	0.110258E-03
10	5	0.106618E-08
10	6	0.398774E-03
10	7	0.396754E-08
10	8	0.207974E-02
10	9	0.451552E-07
10	10	0.639861

1 Quantum wave solution for cond. band valley
0.336204151272744 ->Barrier height

```

6.874429510914734E-002  ->Potential bottom
0.225392217040093      ->Ref. energy
(Energy subbands) - (Ref. energy)
  1  0.355489E-01
  2  0.361585E-01
  3  0.371559E-01
  4  0.385139E-01
  5  0.401954E-01
  6  0.421548E-01
  7  0.443393E-01
  8  0.466902E-01
  9  0.491450E-01
 10  0.516390E-01

      1 Quantum wave solution for val. band valley
0.597696281769814      ->Barrier height
-0.344328580889007     ->Potential bottom
-0.916265928715316     ->Ref. energy
(Energy subbands) - (Ref. energy)
 11  0.381131
 12  0.381043
 13  0.380899
 14  0.380702
 15  0.380458
 16  0.380174
 17  0.379857
 18  0.379515
 19  0.379158
 20  0.378795

=====Start QM Wave Solver==jc jv=>          1          2
      0 Number of 2nd-set states to be searched
Overlaps between cond. and val. subbands
      10          10
  1   1  0.905420
  1   2  0.324795E-08
  1   3  0.622784E-05
  1   4  0.560735E-09
  1   5  0.157094E-05
  1   6  0.253748E-09
  1   7  0.556710E-06
  1   8  0.149108E-09
  1   9  0.206362E-06
  1  10  0.634240E-11
  2   1  0.318201E-08

```

2	2	0.904999
2	3	0.105389E-07
2	4	0.192723E-04
2	5	0.183007E-08
2	6	0.474996E-05
2	7	0.855821E-09
2	8	0.164235E-05
2	9	0.505944E-09
2	10	0.128392E-10
3	1	0.827102E-05
3	2	0.101674E-07
3	3	0.904296
3	4	0.214210E-07
3	5	0.381330E-04
3	6	0.363574E-08
3	7	0.892387E-05
3	8	0.169679E-08
3	9	0.296484E-05
3	10	0.707574E-10
4	1	0.455098E-09
4	2	0.290897E-04
4	3	0.203889E-07
4	4	0.903309
4	5	0.355831E-07
4	6	0.638804E-04
4	7	0.589841E-08
4	8	0.141923E-04
4	9	0.270542E-08
4	10	0.603485E-10
5	1	0.342836E-05
5	2	0.136325E-08
5	3	0.646755E-04
5	4	0.334784E-07
5	5	0.902036
5	6	0.524371E-07
5	7	0.984455E-04
5	8	0.850188E-08
5	9	0.209128E-04
5	10	0.314970E-09
6	1	0.151837E-09
6	2	0.129457E-04
6	3	0.248799E-08
6	4	0.120015E-03

6	5	0.488669E-07
6	6	0.900474
6	7	0.709818E-07
6	8	0.144466E-03
6	9	0.112617E-07
6	10	0.197316E-09
7	1	0.242947E-05
7	2	0.439253E-09
7	3	0.295462E-04
7	4	0.370764E-08
7	5	0.201652E-03
7	6	0.656526E-07
7	7	0.898621
7	8	0.896889E-07
7	9	0.205061E-03
7	10	0.161853E-08
8	1	0.567853E-10
8	2	0.965649E-05
8	3	0.743242E-09
8	4	0.552728E-04
8	5	0.490093E-08
8	6	0.317404E-03
8	7	0.824603E-07
8	8	0.896476
8	9	0.106497E-06
8	10	0.128320E-08
9	1	0.213172E-05
9	2	0.150079E-09
9	3	0.224442E-04
9	4	0.100127E-08
9	5	0.925306E-04
9	6	0.592643E-08
9	7	0.475643E-03
9	8	0.973440E-07
9	9	0.894047
9	10	0.434010E-07
10	1	0.176129E-10
10	2	0.863971E-05
10	3	0.219942E-09
10	4	0.419171E-04
10	5	0.116661E-08
10	6	0.143567E-03
10	7	0.662176E-08

```

10      8  0.683494E-03
10      9  0.107992E-06
10     10  0.454205E-05

      1 Quantum wave solution for cond. band valley
0.336204151272744      ->Barrier height
6.874429510914734E-002 ->Potential bottom
0.225392217040093      ->Ref. energy
(Energy subbands) - (Ref. energy)
  1  0.355489E-01
  2  0.361585E-01
  3  0.371559E-01
  4  0.385139E-01
  5  0.401954E-01
  6  0.421548E-01
  7  0.443393E-01
  8  0.466902E-01
  9  0.491450E-01
 10  0.516390E-01

      2 Quantum wave solution for val. band valley
0.431535240128279      ->Barrier height
-0.510456383168168      ->Potential bottom
-0.622813781415692      ->Ref. energy
(Energy subbands) - (Ref. energy)
 11 -0.635723E-01
 12 -0.640740E-01
 13 -0.648946E-01
 14 -0.660114E-01
 15 -0.673935E-01
 16 -0.690028E-01
 17 -0.707955E-01
 18 -0.727226E-01
 19 -0.747320E-01
 20 -0.764382E-01

=====Start QM Wave Solver==jc jv=>          2          1
      0 Number of 2nd-set states to be searched
Overlaps between cond. and val. subbands
      10          10
  1    1  0.938180E-04
  1    2  0.316970E-10
  1    3  0.100933E-04
  1    4  0.785074E-11
  1    5  0.339313E-05
  1    6  0.341225E-11

```

1	7	0.154847E-05
1	8	0.182898E-11
1	9	0.791915E-06
1	10	0.106050E-11
2	1	0.445538E-08
2	2	0.128919E-04
2	3	0.384835E-09
2	4	0.293580E-05
2	5	0.126454E-09
2	6	0.118462E-05
2	7	0.568598E-10
2	8	0.579190E-06
2	9	0.286172E-10
2	10	0.301873E-06
3	1	0.142736E-03
3	2	0.769774E-09
3	3	0.511432E-05
3	4	0.151220E-09
3	5	0.160839E-05
3	6	0.587510E-10
3	7	0.720806E-06
3	8	0.279775E-10
3	9	0.365865E-06
3	10	0.142188E-10
4	1	0.143433E-05
4	2	0.477395E-12
4	3	0.154140E-06
4	4	0.118231E-12
4	5	0.517804E-07
4	6	0.513096E-13
4	7	0.236066E-07
4	8	0.274393E-13
4	9	0.120581E-07
4	10	0.158653E-13
5	1	0.680240E-10
5	2	0.196589E-06
5	3	0.586921E-11
5	4	0.447479E-07
5	5	0.192748E-11
5	6	0.180409E-07
5	7	0.866051E-12
5	8	0.881092E-08
5	9	0.435511E-12

5	10	0.458635E-08
6	1	0.433715E-11
6	2	0.826810E-04
6	3	0.346673E-14
6	4	0.127903E-04
6	5	0.145836E-13
6	6	0.484845E-05
6	7	0.284709E-13
6	8	0.232065E-05
6	9	0.408342E-13
6	10	0.119786E-05
7	1	0.217779E-05
7	2	0.117687E-10
7	3	0.779948E-07
7	4	0.231022E-11
7	5	0.245107E-07
7	6	0.896873E-12
7	7	0.109736E-07
7	8	0.426722E-12
7	9	0.556315E-08
7	10	0.216674E-12
8	1	0.673128E-13
8	2	0.126165E-05
8	3	0.600224E-16
8	4	0.195068E-06
8	5	0.223716E-15
8	6	0.738817E-07
8	7	0.425982E-15
8	8	0.353233E-07
8	9	0.603885E-15
8	10	0.182096E-07
9	1	0.867513E-04
9	2	0.239408E-08
9	3	0.965404E-05
9	4	0.216144E-09
9	5	0.240739E-05
9	6	0.762106E-10
9	7	0.101985E-05
9	8	0.353188E-10
9	9	0.506564E-06
9	10	0.177786E-10
10	1	0.132389E-05
10	2	0.365046E-10


```

10    3  0.147304E-06
10    4  0.329501E-11
10    5  0.367077E-07
10    6  0.116122E-11
10    7  0.155354E-07
10    8  0.537818E-12
10    9  0.770723E-08
10   10  0.270535E-12

      2  Quantum wave solution for cond. band valley
0.861670969634499      ->Barrier height
0.306942126694649      ->Potential bottom
0.505437215820093      ->Ref. energy
(Energy subbands) - (Ref. energy)
  1 -0.195980
  2 -0.195966
  3 -0.195925
  4 -0.195904
  5 -0.195891
  6 -0.195863
  7 -0.195850
  8 -0.195788
  9 -0.195762
 10 -0.195687

      1  Quantum wave solution for val. band valley
0.597696281769814      ->Barrier height
-0.344328580889007      ->Potential bottom
-0.916265928715316      ->Ref. energy
(Energy subbands) - (Ref. energy)
 11  0.381131
 12  0.381043
 13  0.380899
 14  0.380702
 15  0.380458
 16  0.380174
 17  0.379857
 18  0.379515
 19  0.379158
 20  0.378795

```

Post-Processing of box.qdd File

Without context, the subband energies shown in the box.qdd file provide no usable information. Fig. 8.5 can be used as a reference guide to understand the nomenclature of the box.qdd files to

process these values and yield subband energies and transition energies in eV. This process was automated in code written by S. W. Schaefer.

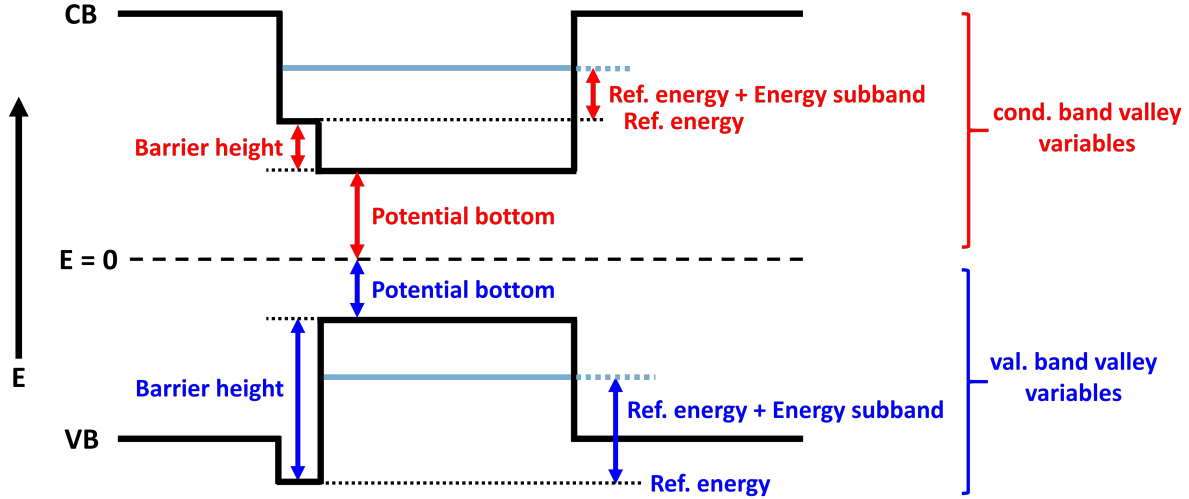


Figure 8.5: Reference guide for processing box.qdd information.

8.4 $\mathbf{k} \cdot \mathbf{p}$ Method for Determining Band Structure

8.4.1 General $\mathbf{k} \cdot \mathbf{p}$ Theory and Background

The simulations described in this thesis use a parabolic band approximation. This is utilized for its simplicity and conciseness, however more complicated theories better represent what occurs in the system. The $\mathbf{k} \cdot \mathbf{p}$ method can also be used to solve for the band structure of our heterostructure. Crosslight currently implements this method for its quantum well structures, but not for more complicated low-dimensional systems. The following theory is extracted from S. L. Chuang's Physics of Photonics Devices [42], and is what Crosslight follows closely for its QW simulations. The $\mathbf{k} \cdot \mathbf{p}$ method is a way to approximate the band structure of semiconductors by using Bloch's theorem to expand the Schrödinger equation around a specific value of $\mathbf{k}$. It's most useful as an approximation for small $\mathbf{k}$ (small deviation away from the band edges), and is also useful for III-V direct band semiconductors.

To understand the principle of $\mathbf{k} \cdot \mathbf{p}$ theory, we begin by presenting the Schrödinger equation for an electron in a periodic potential $V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R})$. Here, the periodic potential is the crystal lattice, and $\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$, where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the lattice vectors and n_1, n_2, n_3 are

integers.

$$H\Psi(\mathbf{r}) = \left(\frac{\hbar^2}{2m_0} \nabla^2 + V(\mathbf{r}) \right) \Psi(\mathbf{r}) = E(\mathbf{k})\Psi(\mathbf{r}) \quad (25)$$

Bloch's theorem depicts the general solution for the above equation:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \quad (26)$$

with

$$u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r}) \quad (27)$$

Rewriting the Schrödinger equation in terms of our Bloch functions, the momentum operator, $\mathbf{p} = -i\hbar\nabla$, and for the n th band with wavevector $\mathbf{k}$ we get:

$$\left(\frac{p^2}{2m_0} + V(\mathbf{r}) \right) \psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) \psi_{n\mathbf{k}}(\mathbf{r}) \quad (28)$$

Expanding this out with the above expression for the electron wavefunction:

$$\left(\frac{p^2}{2m_0} + V(\mathbf{r}) \right) e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \quad (29)$$

$$\frac{p^2}{2m_0} u_{n\mathbf{k}}(\mathbf{r}) + \frac{\hbar}{m_0} (\mathbf{k} \cdot \mathbf{p}) u_{n\mathbf{k}}(\mathbf{r}) + \frac{\hbar^2 k^2}{2m_0} u_{n\mathbf{k}}(\mathbf{r}) + V(\mathbf{r}) u_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) u_{n\mathbf{k}}(\mathbf{r}) \quad (30)$$

$$\left(\frac{p^2}{2m_0} + \frac{\hbar}{m_0} (\mathbf{k} \cdot \mathbf{p}) + V(\mathbf{r}) \right) u_{n\mathbf{k}}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0} \right) u_{n\mathbf{k}}(\mathbf{r}) \quad (31)$$

We define two separate terms here, the first being our unperturbed Hamiltonian as the portion of the above equation relating to electron motion in a periodic potential, independent of $\mathbf{k}$ (or, the $k_0 = 0$ case): $H_0 = \frac{p^2}{2m_0} + V(\mathbf{r})$. The second is the $\mathbf{k} \cdot \mathbf{p}$ term corresponding to the $\mathbf{k}$ -dependent perturbation $H_k = \frac{\hbar^2}{m_0} (\mathbf{k} \cdot \mathbf{p}) + \frac{\hbar^2 k^2}{2m_0}$. This gives us a tidy equation for the modified Hamiltonian displaying the $\mathbf{k} \cdot \mathbf{p}$ term that gives this theory its name:

$$\left(H_0 + \frac{\hbar^2}{m_0} \mathbf{k} \cdot \mathbf{p} \right) u_{n\mathbf{k}}(\mathbf{r}) = \left(E_n(\mathbf{k}) - \frac{\hbar^2 k^2}{2m_0} \right) u_{n\mathbf{k}}(\mathbf{r}) \quad (32)$$

8.4.2 4×4 $\mathbf{k}\cdot\mathbf{p}$ Theory

The Luttinger-Kohn model is a special case of $\mathbf{k}\cdot\mathbf{p}$ method looking at degenerate multibands, where either the 4×4 or 6×6 Hamiltonian matrix can be used. These refer to the number of matrix elements that make up the Luttinger-Kohn (L-K) Hamiltonian describing the total energy of the system. The full Hamiltonian is the 6×6 matrix, which takes into account the LH, HH, and SO bands (doubly degenerate). The LH and HH bands are typically closer to the CB, whereas the SO band is separated by hundreds of millielectron volts from the other two VBs in III-IV semiconductors; for the purposes of these simulations, the 4×4 $\mathbf{k}\cdot\mathbf{p}$ method suffices. Describing a system with 4×4 $\mathbf{k}\cdot\mathbf{p}$ uses the 4×4 L-K Hamiltonian and does not take into account the spin-orbit coupling which induces the SO band. The 4×4 L-K Hamiltonian can also be modified to include the effect of lattice strain on the band edge energies. To understand what each of the terms in the Hamiltonian correspond to, we must define our strain parameters that characterize strain within a three-dimensional lattice using Cartesian coordinates.

$$H = - \begin{bmatrix} P+Q & -S & R & 0 \\ -S^+ & P-Q & 0 & R \\ R^+ & 0 & P-Q & S \\ 0 & R^+ & S^+ & P-Q \end{bmatrix} \quad (33)$$

with basis vectors

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle, \left| \frac{3}{2}, \frac{1}{2} \right\rangle, \left| \frac{3}{2}, -\frac{1}{2} \right\rangle, \left| \frac{3}{2}, -\frac{3}{2} \right\rangle \quad (34)$$

The basis vectors correspond to the LH (with $\pm \frac{1}{2}$ terms) and HH bands (with $\pm \frac{3}{2}$ terms).

If we define our undeformed crystal lattice with $\hat{x}, \hat{y}$ and $\hat{z}$, then we can define unit vectors for our uniformly deformed crystal with directional strain parameters:

$$\mathbf{x}' = (1 + \epsilon_{xx})\hat{x} + \epsilon_{xy}\hat{y} + \epsilon_{xz}\hat{z} \quad (35)$$

$$\mathbf{y}' = \epsilon_{yx}\hat{x} + (1 + \epsilon_{yy})\hat{y} + \epsilon_{yz}\hat{z} \quad (36)$$

$$\mathbf{z}' = \epsilon_{zx}\hat{x} + \epsilon_{zy}\hat{y} + (1 - \epsilon_{zz})\hat{z} \quad (37)$$

Now we can explain all our terms in the 4×4 L-K Hamiltonian shown above:

$$P = P_k(k_x, k_y, k_z) + P_\epsilon(\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}) \quad (38)$$

$$Q = Q_k(k_x, k_y, k_z) + Q_\varepsilon(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}) \quad (39)$$

$$R = R_k(k_x, k_y) + R_\varepsilon(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy}) \quad (40)$$

$$S = S_k(k_x, k_y, k_z) + S_\varepsilon(\varepsilon_{xz}, \varepsilon_{yz}) \quad (41)$$

All of these terms have full expressions that come from the full derivation of the L-K Hamiltonian. It should be noted that P, Q, R, and S all have a k term and an ε term representing the crystal momentum effect and the strain effect on the total energy of the system. This would be a potential extension of the current model for better representation of coupling between the HH and LH bands, also known as valence-band intermixing.

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