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Moving Toward Nano-TCAD Through Multimillion-Atom Quantum-Dot Simulations Matching Experimental Data

Muhammad Usman, Student Member, IEEE, Hoon Ryu, Insoo Woo, David S. Ebert, Senior Member, IEEE, and Gerhard Klimeck, Senior Member, IEEE

Abstract—Low-loss optical communication requires light sources at 1.5 µm wavelengths. Experiments showed, without much theoretical guidance, that InAs/GaAs quantum dots (QDs) may be tuned to such wavelengths by adjusting the In fraction in an In$_x$Ga$_{1-x}$As strain-reducing capping layer. In this paper, systematic multimillion-atom electronic structure calculations explain, qualitatively and quantitatively, for the first time, available experimental data. The nanoelectronic modeling NEMO 3-D simulations treat strain in a 15-million-atom system and electronic structure in a subset of ~9 million atoms using the experimentally given nominal geometries, and without further parameter adjustments, the simulations match the nonlinear behavior of experimental data very closely. With the match to experimental data and the availability of internal model quantities, significant insight can be gained through mapping to reduced-order models and their relative importance. We can also demonstrate that starting from simple models has, in the past, led to the wrong conclusions. The critical new insight presented here is that the QD changes its shape. The quantitative simulation agreement with experiment, without any material or geometry parameter adjustment in a general atomistic tool, leads us to believe that the era of nanotechnology computer-aided design is approaching. NEMO 3-D will be released on nanoHUB.org, where the community can duplicate and expand the results presented here through interactive simulations.

Index Terms—Aspect ratio (AR), quantum dots (QDs), strain, strain reducing layer, wave function, wavelength.

I. INTRODUCTION AND METHOD

Quantum dots (QDs) grown by self-assembly are typically constructed by 50 000 to 10 000 000 atoms, which confine a small, countable number of extra electrons or holes in a space that is comparable in size to the electron wavelength. Under such conditions, QDs can be interpreted as artificial atoms that can be custom-tailored to new functionality. As such, these structures have attracted significant experimental and theoretical attention in the field of nanoscience [1]–[3]. The new and tunable optical and electrical properties of these artificial atoms have been proposed in a variety of different fields, for example, in communication and computing systems, medical, and quantum computing applications. Predictive and quantitative modeling and simulation may help to narrow down the vast design space to a range that is experimentally affordable and move this part of nanoscience to nanotechnology.

After ten years of development, we demonstrate here the capabilities of the nanoelectronic modeling NEMO 3-D tool kit that can now quantitatively model complex sequence of multiple experiments without any model parameter adjustments. Input to the calculations are the previously published atomistic material parameters, and the experimental device geometries and alloy concentrations. The resulting numerical simulation domain includes around 15 million atoms to represent the realistic device. Quantitative agreement of the simulations with a nonlinear behavior across a sequence of different experimental devices is found. The internal model variables such as strain, atom positions, and disorder can subsequently be used to gain physical insight and intuition into the competing processes observed experimentally by mapping into simplified models. It is, however, critical to start from the full atomistic model in order to include the important effects initially, rather than trying to access the relative importance of the simple models. It is shown that starting from the simple models has, in the past, led to wrong conclusions.

Fig. 1 shows two views of the atomistically represented QD system. An InAs dome-shaped QD is grown on top of an InAs wetting layer and covered with an In$_{0.4}$Ga$_{0.6}$As [Fig. 1(a)] or In$_{0.4}$Al$_{0.6}$As [Fig. 1(b)] capping layer, followed by a GaAs cap. The regularly distributed “As” atoms are not shown for clarity. The atomic disorder in the alloyed capping layer as well as the InAs QD interface is evident. The In fraction $x$ in the In$_x$Ga$_{1-x}$As cap layer has been varied in experiments to tune the optical emission spectrum without much theoretical guidance. The NEMO 3-D simulation is based on this atomistic device representation and intrinsically incorporates the disordered atom placement, and our model can explain the observed experiment nonlinear behavior without any parameter adjustments.

In recent years, much interest has been focused on GaAs-based optical devices used for optical-fiber-based communication systems at longer wavelengths (1.3–1.5 µm). Several experimental groups have tried to achieve emissions at...
wavelengths above 1.3 μm either by using GaInNAs QDs in a GaAs matrix [4], [5] or by embedding InAs QDs in a In$_x$Ga$_{1-x}$As strain-reducing capping layer (SRCL) [6]–[11]. To date, there is not much theoretical analysis of SRCL-capped systems available in the literature, and the dependence of emitted spectra wavelength on the In fraction and the thickness of the SRCL has not been studied in detail. The effect of a graded interface between the QD and the surrounding buffer as well as QD size variations has not been investigated yet either. An eight-band k-p method was used in [19] to explain the observed redshift without giving any quantitative contribution of QD size change and reduction of barrier height on SRCL side. A single-band effective mass approximation is used in [8]. That study claims that the reduction of confinement barrier height on the SRCL side is a major source of observed redshift. In this paper, we qualitatively and quantitatively explain the experimentally observed redshift of the emission spectra in terms of the strain relaxation in the growth direction, the change in the volume of the QDs, and the reduction of the barrier height on the SRCL side in contradiction to the reduced-order models used before. Our atomistic tight binding model clarifies the physical picture and shows that this barrier height lowering makes only a very minor contribution to the redshift, in contrast to the explanation of the continuum models. A critical insight needed to solve this problem is the atomistic representation of the system rather than the continuum picture and the subsequent consequences of the atomistic representation on the electronic structure. The representation of the bi-modal InAs and GaAs bond lengths turns out to be of critical importance which happens to be completely missing in continuum and k-p methods.

A comprehensive analysis of the strain relaxation, the QD size changes, and the barrier reduction on the SRCL side is presented for strain-reduced QDs using the NEMO 3-D [14], [15], [33]. NEMO 3-D can calculate strain and electronic structure for realistically sized systems as large as 52 million atoms [14], [15], which corresponds to a simulation domain of (101 nm)$^3$. Strain is calculated using an atomistic valence force field (VFF) method [17] and the electronic structure using a 20-band sp$^3$d$^5$s$^*$ nearest neighbor empirical tight binding model [16]. The tight binding parameters are fit to reproduce the bulk properties of GaAs, InAs, AlAs, Si, and Ge with respect to room-temperature band edges, effective masses, hydrostatic/biaxial strain behavior, and relative band edges [16], [35], [40]–[42] using a global minimization procedure based on a genetic algorithm [34] and analytical insight [35]. The strain and electronic structure properties of alloys are faithfully reproduced through an explicit disordered atomistic representation [33], [35] rather than an averaged potential representation. The explicit alloy representation also affords the ability to model device-to-device fluctuations, which are critical in modern decanano devices. The bulk-based atom-to-atom interactions are transferred into nanoscale devices where no significant bond charge redistribution or bond breaking is expected and strain is typically limited to around 8%. To material scientists and ab initio theorists, this model might appear to have a very limited range of validity, but it basically covers all standard semiconductors relevant for realistic devices where bonds and geometries are stable and contain tens of thousands to tens of millions of atoms. In fact, one might argue that a device in which bonds are established and dissolved result in undesirable electronic structure fluctuations for the realistic devices. For realistic semiconducting nanoscale systems, our tight binding approach, employed in NEMO 1-D and NEMO 3-D, has been validated experimentally through:

1) high-bias, high-current, quantitative resonant tunneling diode modeling [36] (unprecedented match to a suite of experimental data of room-temperature quantum effect devices);
2) photoluminescence in InAs nanoparticles [37];
3) modeling of the Stark effect of single P impurities in Si [38] (demonstrating the need to include an atomistic representation rather than continuum effective mass models);
4) distinguishing P and As impurities in ultrascaled FinFET devices [46], [48];
5) the valley splitting in miscut Si quantum wells on SiGe substrate [39] (demonstrating importance of the atomistic wafer step disorder and alloy disorder in SiGe).

In this paper, NEMO 3-D is used as an analysis-and-design tool without any material parameter tuning. Semianalytical, reduced-order models are used to provide insight into the meaning and validity of the numerical results.
Understanding the effects of strain in an InAs/GaAs system is of critical importance [18], [19], [24]. The introduction of an SRCL modifies the strain distributions significantly, and the hydrostatic and the biaxial strain relaxations for varying In fractions in the SRCL surrounding the InAs QD need to be studied. It is shown that strain relaxation inside the InAs QD has a significant contribution in the observed redshift of emission spectra for small In concentrations ($x < 0.2$). For large In fractions ($x > 0.2$), another physical modification in the system begins to play a major role in the additional redshift. The physical shape of the QD changes where a decrease in the base length and a relatively larger increase in the height of the InAs QD modify the quantum confinement, and therefore, change the confinement energy. The two strain-induced effects of band edge changes and shape changes are mixed nonlinearly due to differing In–As and Ga–As bond lengths of the atomistically disordered InGaAs buffer system. NEMO 3-D includes all these effects due to its fundamental atomistic material representations and faithfully reproduces the experimentally observed [6] nonlinear behavior of the emission wavelength as a function of In concentration. Simple effective mass models of this system predict [8] that the introduction of the InGaAs buffer reduces the electronic confinement potential relative to the GaAs buffer. Our atomistic simulations show that this effect does not take place by direct comparison to an InAlAs buffer, which has the same strain but different electronic structure behavior as the InGaAs buffer.

Significant nonlinearity in the biaxial strain components can be attributed to the bimodal In–As and Ga–As bond distributions in InGaAs that can only be captured by an atomistic representation. Additional case studies show that the nonlinearity in the optical wavelength tuning profile is stable relative to experimentally unavoidable effects such as interface interdiffusion (interface softness) and QD size variations.

NEMO 3-D can be used to gain fundamental insight into the key physics and guide future experiments with modest computational expense and time at about 10 h on 60 CPUs per simulation. Efforts are under way to enable anyone in the community to perform these NEMO 3-D simulations on nanoHUB.org [30] that already hosts over 130 nanosimulation tools, including an educational version [49] of NEMO 3-D. A full-capability NEMO 3-D release is planned for the fall of 2009. The educational NEMO 3-D version entitled “Quantum Dot Lab” runs in a few seconds and has been used by over 1600 users who ran over 14 000 simulations.

II. SIMULATED SYSTEM AND MATCH TO EXPERIMENT

Fig. 2(a) shows the schematic of the simulated system that consists of a dome-shaped InAs QD of 5 nm height and 20 nm base diameter on a 1 monolayer (ML) InAs wetting layer. The QD is embedded in an In$_x$Ga$_{1-x}$As SRCL of height “D” nanometer. A large GaAs buffer (a total volume of $60 \times 60 \times 66$ nm$^3$) surrounds the whole structure containing 15.2 million atoms, which is used for the atomistic strain calculation. Physical intuition tells us that the states of interest are confined in the region around the QD. Numerical experiments confirm that the electronic structure computation can be performed in a smaller region (50 nm in the lateral dimension and 56 nm in the growth direction consisting of 8.96 million atoms) around the InAs QD without any loss of accuracy, after the atom positions have been computed in the large domain, due to the long-range strain interaction. Two different values of $D$ are considered: $D = 5$ nm and $D = 10$ nm, subsequently labeled D5 and D10, respectively. These systems are the nominal topologies given in the experiments [6], [7]. The In fractions ($x$) in the SRCL take the values of 0 (no capping layer), 0.12, 0.18, 0.28, 0.4, and 0.45.

Fig. 2(b) compares the optical emission wavelength observed in a complex experimental [6] (dotted curves) device sequence against NEMO 3-D simulations (triangles). The three experimental curves are obtained at different growth conditions, resulting in nominally identical dots of average diameter of 20 nm and height of 5 nm. The NEMO 3-D simulations take as input parameters the geometry and alloy compositions, as described in the experimental publications, without any other material parameter or geometry adjustments. Previously published material parameters [16] are used and no parameters other than the QD size, wetting layer thickness, and the alloy composition are entered. A surprisingly good agreement between the experimental results and the “out-of-box” NEMO 3-D calculations is observed. If this were production-level, conventional nanotechnology computer-aided design (nano-CAD) engineering work, one might conclude that NEMO 3-D is a tool that can be used to explore this design space quantitatively. We will soon release this code on nanoHUB.org [30].

The experiment and simulations show an interesting nonlinear behavior whose origin is not clearly understood. The remainder of this paper reveals the intriguing details that lead to this complex nonlinear behavior and provides insights into the physical problem through analysis of internal model variables and
derived simplified analytical models. The critical insights gained from this study are the following.

1) Qualitative and quantitative explanation of physics:
   a) atomistic material representation includes bimodal In–As and Ga–As bond lengths:
      ➔ nonlinear strain distribution as a function of In concentration;
   b) strain relaxation in growth direction:
      ➔ redshift of emission spectra;
   c) QD shape changes [aspect ratio (AR)]:
      ➔ redshift of emission spectra;
   d) changes in electronic confinement of the InGaAs buffer barrier height:
      ➔ negligible contribution to change in emission spectra;
   e) atomistic interface detail:
      ➔ softness of QD boundary causes a small blue shift;
   f) QD size variations:
      ➔ little effect on conclusions can provide guidance to device design.

2) Conceptual observations and conclusions:
   a) details of atomistic strain and electronic calculations are important:
      ➔ effective mass models and continuum theories lead to wrong conclusions;
   b) NEMO 3-D electronic structure at room temperature matches experiments more closely than pseudopotential method for the InGaAs system (confinement energies and badgaps);
   c) NEMO 3-D matches experimental InAs/GaAs QD data out-of-box without any parameter adjustments, like NEMO 1-D ten years earlier [47] for InP- and GaAs-based resonant tunneling diodes:
      ➔ nano-TCAD is approaching for QD systems.

III. RESULTS AND DISCUSSION

A. Strain Relaxation Impact

Fig. 3 shows the hydrostatic \( \{ \varepsilon_{xx} = \varepsilon_{yy} + \varepsilon_{zz} \} \) and the biaxial strain \( \{ \varepsilon_{xx} = \varepsilon_{yy} - 2\varepsilon_{zz} \} \) components [21] for different In fractions and heights of the SRCL. Only the spatial regions around the central QD are shown for clarity. The actual device simulation domain is significantly larger [Fig. 2(a)], where the substrate and lateral strain have decayed. The hydrostatic strain is strictly negative everywhere, large only within the InAs QD, and almost zero outside. The larger bond length InAs QD is compressed by the smaller bond length GaAs environment in the lateral direction. The peak value variation of the hydrostatic strain within the InAs QD in the [0 0 1] and [1 0 0] directions are shown at the bottom of the left column of Fig. 3. As the In fraction \( (x) \) increases from 0 to 0.4, the hydrostatic strain decreases and the peak value of the strain shifts from the top toward the center of the dot. This shift of the peak hydrostatic strain in the [0 0 1] direction results in a change of the sign of the strain gradient near the top of the dot.

The biaxial strain shows more prominent effects with the increased In fraction. The biaxial strain is negative within the dot and positive outside the dot penetrating deep inside the GaAs buffer from the top and the bottom dot boundaries. A strong vertical dominance of the biaxial strain field is evident in the absence of SRCL, while the strain does not penetrate as deeply into the lateral directions. In the lateral direction, only the wetting layer shows larger biaxial components (as expected). The introduction of the SRCL appears to spread the biaxial strain further in the lateral direction. This is indeed evident with the line cuts of the biaxial strain through the center of the dot in the

Fig. 3. Hydrostatic \( \{ \varepsilon_{xx} = \varepsilon_{yy} + \varepsilon_{zz} \} \) (left column) and biaxial strain \( \{ \varepsilon_{xx} + \varepsilon_{yy} - 2\varepsilon_{zz} \} \) (right column) for In fraction \( (x) \) of 0, 0.18, and 0.4 in D5 and D10 in the spatial region around the QD. Even qualitatively, the InGaAs SRCL creates a reduction in the biaxial fringing strain fields. The last two rows show the peak hydrostatic strain (left) and the biaxial strain (right) along the [0 0 1] (upper row) and [1 0 0] (lower row) directions through the center of the InAs QD as a function of distance in D5. The arrows are placed to guide the eyes for changes with increasing \( x \). In [0 0 1] direction, the hydrostatic strain profile peak moves to the center of the QD making the strain profile a bit more symmetric toward the center as the In fraction increases. With the same In fraction increase, a reduction of the biaxial strain around the QD and an increase inside the QD are observed in [0 0 1] direction. Line plots along [1 0 0] direction show that the SRCL spreads the hydrostatic and biaxial strains significantly in the lateral direction. Dotted line shows the average value of strain calculated in a window of 10 nm around each point. A nearly constant 5% biaxial strain is observed throughout the SRCL buffer. The biaxial strain decrease outside and increase inside point to a strong AR distortion inside the dot.
Fig. 4. (a)–(d) Band edge diagrams along the [0 0 1] (growth) direction through the center of InAs QD for the In fractions \( x \) of 0, 0.12, 0.18, and 0.4 in \( D5 \). In each diagram, the binding energy of the first electron and the hole levels, the electronic bandgap measured at the center of InAs QD, the optical bandgap, and HH/LH splitting inside and outside the QD are shown. As the In fraction of SRCL increase, the bandgaps shrink, and hence, a redshift of emission spectra can be predicted. (e) CB, HH, and LH curves are reproduced from (a), (b), (c), and (d). Arrows are marked to indicate the direction of change in the band edges.

lateral direction (see Fig. 3, last row). Dotted line shows average strain in the buffer region. Fig. 3 shows a nearly constant \( \sim 5\% \) strain throughout the SRCL layer. As the dot is surrounded by the In\(_x\)Ga\(_{1-x}\)As SRCL, the positive strain outside the QD decreases in the vertical direction and the negative strain inside the dot increases. The biaxial strain strongly affects the hole confinement potentials \([18],[21]\), and therefore, a reduced heavy hole (HH) and light hole (LH) splitting outside the dot and an increase (decrease) of the well depths for the HH (LH) will be observed.

The speckles in the SRCL region indicate the inhomogeneous nature of the strain in the InGaAs region, which is due to the bimodal In–As and Ga–As bond length distributions that have been observed experimentally \([45]\), and are faithfully reproduced in NEMO 3-D \([33]\). While biaxial component fringe fields are visible in the QD without an SRCL, the increasing In fraction in the SRCL appears to smooth out these fringe fields and homogenize the biaxial stain inside the QD.

In Fig. 3, we notice that the hydrostatic strain has a peak value of \( \sim -0.094 \) and the biaxial strain has a peak value of \( \sim -0.23 \) for \( x = 0.4 \) within the QD region. Here, we want to point out that our InAs tight binding parameters have been matched against Van de Walle \([23]\) reference data for the hydrostatic and biaxial strains of \( \sim -0.21 \) and \( \sim -0.29 \), respectively. The InAs conduction band, HH band, LH band, and split-off band edges for a peak hydrostatic strain of \( \sim -0.21 \) (\( \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = -0.07 \)) and a peak biaxial strain of \( \sim -0.29 \) (\( \varepsilon_{xx} = \varepsilon_{yy} = -0.07, \varepsilon_{zz} = -1.084, \) and \( \varepsilon_{xx} = 0.075 \)) are plotted in \([33, Fig. 7]\). Our \( sp^3d^5s^* \) band edges closely matched with the reference data from Van de Walle.

Fig. 4 shows the local band edge diagrams for the lowest conduction band and the top three hole bands (HH, LH, and split off) for \( x = 0, 0.12, 0.18, \) and 0.4 in \( D5 \) along the central line through the dot along the growth direction. Also shown are the first few confined states in the conduction and the valence bands. The optical gaps and the electronic gaps are marked on each diagram. The spatial variations in the local band edges indicate strong influence by the hydrostatic and the biaxial strain profiles.

A simplified model \([20]\) can partially explain the strain effects. The strained electron confinement potential is determined by the hydrostatic strain \((1)\) and the strained hole confinement potentials are determined by both the hydrostatic and the biaxial strains \((2) \) and \((3)\)

\[
\delta E_C = a_e \varepsilon_H 
\]

\[
\delta E_{HH} = a_e \varepsilon_H + \frac{b_e \varepsilon_B}{2} 
\]

\[
\delta E_{LH} = a_e \varepsilon_H - \frac{b_e \varepsilon_B}{2}. 
\]
The hydrostatic and the biaxial deformation potential values for the InAs \((\alpha_v = -5.08 \text{ eV}, \alpha_h = 1.0 \text{ eV}, \text{ and } b_v = -1.8 \text{ eV})\) are well documented in the literature [23]. As the In fraction of the SRCL increases, the negative hydrostatic strain decreases in magnitude, reducing the positive \(\delta E_{C}\) and shifting the conduction band down. The hydrostatic component of the strain-induced bandshift for the HH and LH bands induces a negative \(\alpha_v, \epsilon_d \) and the reduction of \(\epsilon_d\) shifts the bands up. The biaxial strain component, however, has opposite trends for the HH and the LH band edges. The increase in the negative biaxial strain \(\epsilon_B\) inside the QD creates a positive \(b_v \epsilon_B / 2\), and therefore, shifts the HH band up in energy and the LH band down in energy. Hence, for the HH band edge, the biaxial and the hydrostatic strain effects accumulate, whereas for the LH band edge, they tend to cancel each other. For \(x = 0.4\), the biaxial strain effect dominates significantly over the hydrostatic strain effect and a significant change in the shape of the local LH and HH band edges can be observed.

The hydrostatic strain reduction directly shifts the electron band edge downward and it shifts HH band edges upward inside the InAs QD. The splitting between the HH and LH bands in the center of the dot increases with increasing In fraction from 146.9 to 598.4 meV. Since the biaxial strain has the opposite sign outside of the QD and decreases with increasing In fraction, the trend in the HH and LH splitting has an opposite trend outside of the QD and the energy splitting is seen to decrease from 221.4 down to 145.5 meV as the In fraction increases. Overall, the LH band is shifted away from the centrally relevant energies and appears to be less important in these devices. The highest confined hole states can be expected to be primarily HH-based, showing strong confinement to the QD region.

Fig. 3 shows that the biaxial strain relaxation due to SRCL results in an increase (decrease) of the magnitude of the negative (positive) strain inside (outside) the InAs QD with increasing \(x\). Since the biaxial strain is responsible for the LH and the HH band splitting [18], this increase (decrease) of the biaxial strain magnitude results in enhanced (reduced) splitting of the LH and the HH band offsets inside (outside) the QD, as evident in Fig. 4. From \(x = 0\) to \(x = 0.4\), a \(\sim 452 = 598.4 - 146.9\) meV \((\sim 75.4 = 221.4 - 145.5\) meV) increase (decrease) in the splitting between HH and LH bands is calculated from the strain-modified band edges. Similar effects have been observed in [17]. This increased separation of HH–LH bands causes the highest confined states to be more and more HH-like states, which will bind these states closer and closer to the center of the QD and lessens the penetration into the barrier.

Fig. 4 shows the binding energies for the ground electron and hole energy levels. We calculate electron binding energy of \(\sim 152\) meV and hole binding energy of \(\sim 258\) meV for \(x = 0\) in D5. Our hole binding energies are in good agreement with experimental measurements of Itskевич et al. [27] \((\sim 250\) meV) and Berryman et al. [28] \((\sim 240\) meV) at room temperature for similar sized QDs. As an additional verification for our electron binding energy, we point to another experiment. Tang et al. [26] reported an electron binding of \(\sim 80\) meV for a QD with an estimated base diameter of 13–17 nm. For a base diameter of 15 nm and height of 3.5 nm, we calculate an electron binding energy of \(\sim 91\) meV. This agreement with experimental electron and hole binding energies quantitatively validates the NEMO 3-D simulation capabilities.

A similar QD system was simulated in [25] using an atomistic pseudopotential method. Using a QD base diameter of 25.2 nm and QD height of 3.5 nm, the authors reported the electron and hole binding energies as 271 and 193 meV, respectively. We simulate the same sized QD and found that the electron and hole binding energies are \(\sim 181\) and \(\sim 289\) meV, respectively. The pseudopotential calculations for the same sized QD result in electron confinement energies that are too low and hole confinement energies that are too high while our tight-binding NEMO 3-D results are much closer to the experimental values of Berryman et al. [28] and Tang et al. [26]. We attribute the NEMO 3-D agreement with technologically relevant room-temperature data to the intensive tuning efforts [16], [33]–[35] of the InAs and GaAs constituent materials to available experimental room temperature bulk data. Another critical advantage of a local basis representation used in NEMO 3-D over a plane-wave basis used in pseudopotentials is that the representation of arbitrarily disordered systems does not require an expert user to tune the number of included plane waves in the system. The computational burden is determined in NEMO 3-D purely by the size of the system, and not the degree of disorder. This has particular relevance for the creation of a nano-TCAD tool to be used by nontheory experts as envisioned for a community on nanoHUB.org.

As a general trend, we observe here that the introduction of the SRCL increases the binding energies with the In fraction \(x\). A 58 meV increase from 152 to 210 meV and a \(\sim 125\) meV increase from \(\sim 258\) to \(\sim 383\) meV in the electron and the hole binding energies, respectively, are calculated from \(x = 0\) to \(x = 0.4\). Fig. 3 shows for \(x = 0.12, 0.18, 0.28, \text{ and } 0.4\) an average hydrostatic strain magnitude reduction of 0.00197, 0.003, 0.0033, and 0.00494, and an average increase in the magnitude of biaxial strain within the QD is 0.01436, 0.018, 0.0508, and 0.064, respectively. Corresponding to these hydrostatic and biaxial strain changes, (1) gives an average change in the strain-modified conduction band edge of 10, 15.25, 16.9, and 25.114 meV and (2) for the HH band edge, a corresponding change of 14.9, 20, 49.09, and 63.29 meV. These changes in the confinement potentials are expected to directly translate into the corresponding changes of the electron and the hole ground state energy levels, and hence, the optical bandgap. However, the simple model predicts, at \(x = 0.4\), a \(\sim 88\) meV (25.114 + 63.29 meV) strain induced redshift of the emission spectra while a \(\sim 183\) meV change of the optical gap is simulated with NEMO 3-D simulation at \(x = 0\) and \(x = 0.4\) in Fig. 4. We therefore conclude that at large values of \(x\), the strain contributes less than half of the overall redshift of the emission spectra. Another physical effect is needed to explain the remaining shift in the emission spectra. In the next section, we will explain the effect of AR variation in the overall redshift of emission spectra.

B. AR Change of the QD

The argument that the hydrostatic and biaxial strain components shift the conduction band and HH band edges, while
and is tensile. The reason is that the QD is flat and the optical absorption energy is not only influenced by the total shift in the optical absorption energy. We show here that the optical absorption energy is not only influenced by the bottom of the conduction band and the top of the valence band but also by the physical shape of the quantization potential.

In the absence of the SRCL, the in-plane strain ($\varepsilon_{xx}$, $\varepsilon_{yy}$) is compressive and the vertical strain ($\varepsilon_{zz}$) is tensile. The reason for the tensile vertical strain ($\varepsilon_{zz}$) is that the QD is flat and the larger in-plane compression results in vertical expansion due to the Poisson effect. Self-assembled InAs QDs form on GaAs to minimize the biaxial strain in the growth layer. Only a thin strongly biaxially strained wetting layer remains. Capping the InAs wetting layer and QD with the InGaAs alloy introduces more In–As bonds into the system that push against the lattice constant imposed by the GaAs substrate. The whole InGaAs SRCL is biaxially compressively strained to accommodate the GaAs substrate. This implies that the InAs QD can no longer compensate by expanding against the GaAs cap, with a smaller lattice constant. The InAs QD must compensate by expansion into the growth direction. Due to these effects, biaxial strain ($\varepsilon_{B}$) inside the QD is increased and hydrostatic strain ($\varepsilon_{H}$) is decreased for increasing $x$ in the SRCL, as shown in Fig. 3. In conclusion, with the introduction of the SRCL, the InAs atoms inside the QD align themselves more closely with the vertical atom planes in the underlying substrate, push less laterally against the surrounding buffer, and compensate the loss of volume by vertical expansion. The QD height increases and the QD width decreases slightly, as shown in the inset of Fig. 5, resulting in a change in AR (height/base) as indicated in Fig. 5. The QD changes shape. Appendix A derives [22] from a very simple particle in a box problem that for low-AR QDs (AR < 0.3), small increases in QD height decrease the bandgap more than a corresponding increase in base length. The following paragraphs elaborate on the effect of the change in the QD shape and relate it quantitatively to the observed change in optical bandgap.

![Fig. 5. Volume of the InAs QD and the AR (height/base) are shown as a function of the In fraction ($x$) in the SRCL in D5. As the In fraction increases, the dot height and the AR increase. Inset shows the base and the height of the InAs QD as a function of the In fraction in the SRCL. As the In fraction increases, the height increases and the base length decreases.](image)

In the presence of the SRCL, the reduction of the base diameter of the InAs QD increases the optical bandgap of the system (a blue shift of the emission spectra). On the other hand, the increase in the height of the InAs QD has the opposite trend: it tends to decrease the optical bandgap of the system (the redshift of the emission spectra). The QDs studied in this paper are the low-AR dome-shaped QDs and are much more sensitive [22] to the height changes as compared to the base diameter changes. The increase in the optical bandgap due to the changes in the base diameter are therefore negligible compared to the decrease in the optical bandgap due to the increase in the height of the QD. As a result, the size changes of the QD in the presence of the SRCL overall contribute in the redshift of the emission spectra. For the large values of the In fraction ($x$), this effect becomes a significant source of the energy shift. From $x = 0$ to $x = 0.4$, it is calculated from the NEMO 3-D simulations (Appendix B) that the AR change causes a red energy shift of $\sim 90$ meV. This is a significant ($\sim 50\%$) contribution in the total optical bandgap shift of $\sim 183$ meV between $x = 0$ and $x = 0.4$.

Our numerical results can be verified through a simple single band effective mass particle in a box model (ignoring the strain effects). It predicts a decrease of $\sim 60$ meV in the optical bandgap for the base and height changes in Fig. 5 (see Appendix A). Fig. 6(b) compares the NEMO 3-D results with the results from simple analytical models. The strain contribution is calculated...
from (1) and (2) and the data from Fig. 6(a). AR contribution is calculated from the data of Fig. 5 and the procedure of Appendix B. The AR contribution shows a strong nonlinear behavior while the strain shows a roughly linear behavior. The total change in the optical emission wavelength calculated from the analytical models shows a nonlinear behavior in a reasonable qualitative agreement with NEMO 3-D results. The simplified model in Appendix A indicates that the AR change of the QD indeed results in a significant change in quantum confinement and that, in turn, changes the bandgap significantly. Clearly, this change in AR is strain-induced, but change in the QD shape is a bit of a surprising effect beyond the typical bandgap change due to strain. This dot shape change would normally not be considered in solid continuum strain and electronic structure models (k-p).

Fig. 6(c) plots the first five electron and (d) the first three hole energy levels as a function of the SRCL In fraction \(x\) for \(D5\) and \(D10\). Three critical physical issues can be extracted from Fig. 6: 1) dependence of SRCL thickness; 2) applicability of lasing devices; and 3) relation of nonlinear biaxial strain and hole energies, as discussed in the three subsequent paragraphs.

Increasing the SRCL thickness \(D\) from 5 to 10 nm does not change the optical gap significantly. At \(x = 0.4\), \(e1(D5) - e1(D10)\) is only 7.5 meV and \(h1(D5) - h1(D10) = 14.3\) meV. This is because once the QD is covered with the In\(_x\)Ga\(_{1-x}\)As SRCL, further increase in the thickness \(D\) does not change the strain relaxation or the QD size much. This effect is also presented in [20].

The energy difference \(e2 - e1\) is quite important for laser applications. This difference should not decrease with increasing SRCL effects to avoid undesirable occupation of higher excited states [8]. Fig. 6(c) shows that this difference (\(\sim 36\) meV) is almost independent of \(x\). Hence, our atomistic tight binding model predicts that the change of the In fraction of the SRCL does not limit the possible use of this device for the long-wavelength laser applications.

The change in electron energy levels is approximately linear with increasing \(x\) corresponding to the linear behavior of the hydrostatic strain in Fig. 6(a) and (1). The hole energy levels show an abrupt jump for \(x\) above 0.18 correlated with the nonlinear behavior of the biaxial strain in Fig. 6(a). Since the hydrostatic strain impact for both electron and hole energy levels is the same [(1)–(3)], this additional change above \(x = 0.18\) can be explained in terms of the biaxial strain component as follows: Fig. 6(a) plots the hydrostatic and biaxial strain as a function of In fraction \(x\) at the center of InAs QD. The hydrostatic strain decrease is almost linear with \(x\). For the In fractions \(x\) above 18\%, a large increase in the negative biaxial strain within the InAs QD contributes in the significant change in the hole confinement potentials and the energy levels.

The origin of the nonlinear behavior of biaxial strain in Fig. 6(a) can be explained in terms of nonlinear change of the bond lengths under strained environment. Fig. 7(a) plots the mean bond lengths of In\(_x\)Ga\(_{1-x}\)As alloy as a function of In composition \(x\). The solid lines are experimentally reported data from Mikkelsen et al. [45] for a bulk In\(_x\)Ga\(_{1-x}\)As alloy and computed data from NEMO 3-D simulations for a bulk In\(_x\)Ga\(_{1-x}\)As alloy [33]. However, when an alloy is placed under strain distortion, the linear nature of bimodal bond length changes. Circles are from NEMO 3-D data for a strained In\(_x\)Ga\(_{1-x}\)As 5-nm-thick quantum well placed on and capped by GaAs. The bond length distribution is still bimodal, however, the In–As and Ga–As curves approximately parallel to each other. The strain applied by the GaAs substrate changes the linear bond length distortion observed in bulk to a behavior virtually independent of In fraction. Similar results were reported in [44].

An analytical model was developed in [43] for strained alloys. We compare our NEMO 3-D results for strained QW [rectangles in Fig. 7(b)] with the analytical model [43] [circles in Fig. 7(b)]. A close qualitative match is found to within 0.73\%, validating the NEMO 3-D model. A critical issue that cannot be resolved with an analytical model is the influence of an embedded QD on the bond distribution. The dotted lines the average crystal bond length within the QD region for a QD placed inside the

![Fig. 7: (a) In–As and Ga–As bond length average as a function of In fraction \(x\). Solid lines correspond to experimental data reported by Mikkelsen and Boyce (1982) and computed data for bulk In\(_x\)Ga\(_{1-x}\)As material reproduced from [33]. Circles are for strained QW (In\(_x\)Ga\(_{1-x}\)As QW inside GaAs buffer) using NEMO-3-D. (b) Mean crystal bond length as a function of In fraction \(x\) of SRCL. Circles are the calculated bond lengths from analytical expressions of [43] for 1-D QW. Rectangles are for NEMO 3-D simulations for 1-D QW. Triangles are for NEMO 3-D simulations including QD inside QW. (c) Average bond lengths as a function of distance along [0 0 1] in D5. A nonlinear change in bond length inside QD can be observed as In fraction is changed from 0 to 0.4.](image-url)
In$_x$Ga$_{1-x}$As alloy ($D5$). The bond lengths increased slightly but have the similar nonlinear trend.

Fig. 7(c) plots the average bond length as a function of distance along [0 0 1] direction through the center of QD in $D5$. Interestingly, the bimodal distribution has a spatial dependence within the QD. Also, we can see the nonlinear change of bond lengths within the QD as $x$ increases from 0 to 0.4. Hence, we conclude that in strained alloys, the linear interpolation of bond length becomes invalid, and an atomistic study is necessary to capture the nonlinear behavior of bond lengths.

Fig. 8(a) repeated from Fig. 2 shows the calculated optical bandgap and the emission wavelength as a function of SRCL In fraction ($x$) in $D5$. The dotted lines are shown from experiments [6]. As the value of $x$ increases, the optical bandgap decreases and the emission wavelength increases. A 1.53 $\mu$m wavelength is calculated for $x = 0.45$, which closely matches the experimental value of 1.52 $\mu$m.

An astonishing agreement with experiment is observed. Here, we again emphasize that there were no adjustments to any material parameters [16] performed in NEMO 3-D to match the experiment. In particular, we note that the simulation quite nicely models the nonlinear behavior of the experimental data.

The earlier sections describe the contribution of the strain and AR variation in the overall redshift of the emission spectra using a simulator based on atomistic tight binding parameters [16]. The strain and AR variations each contribute about half of the energy shift. To validate our results with a simple analytical model, which allows us to understand the results more intuitively.

### Table I

<table>
<thead>
<tr>
<th>Contribution from:</th>
<th>From our Simulations</th>
<th>From calculations of Appendix A</th>
<th>From calculation of Appendix C</th>
</tr>
</thead>
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<tr>
<td>AR variation</td>
<td>~90meV</td>
<td>~60meV</td>
<td>~78meV</td>
</tr>
<tr>
<td>Strain relaxation</td>
<td>~88meV</td>
<td>~52meV*</td>
<td>~66meV</td>
</tr>
<tr>
<td>Total</td>
<td>~178meV</td>
<td>~112meV</td>
<td>~144meV</td>
</tr>
</tbody>
</table>

The later sections describe the contribution of the STRAIN and AR variation in the overall redshift of the emission spectra using a simulator based on atomistic tight binding parameters [16]. The strain and AR variations each contribute about half of the energy shift. To validate our results with a simple analytical model, which allows us to understand the results more intuitively.

### C. Atomistic Interface Effect

Experimentally, it is very hard to find the exact composition of QDs. Particularly, the abrupt interface between InAs QDs and the surrounding GaAs buffer, assumed in most of the literature, may not be true. To investigate the effect of QD interface softness on the emission spectrum, three different samples of QD were simulated. The QD consisted of an inner dome of diameter 18 nm composed of pure In$_x$Ga$_{1-x}$As ($x=1$, InAs material. The dome was then covered by 1-nm-thick layers of each In$_x$Ga$_{1-x}$As and In$_x$Ga$_{1-x}$As [see inset in Fig. 7(b)].

In the first sample $D5^{(1)}$, $x=1$, $x=1$, and $x=1$, $x=0$, and $x=0$ have value of 1. This corresponds to a pure InAs QD that was previously labeled as $D5$. In the second sample $D5^{(2)}$, $x=1$, $x=1$, and $x=3$ all have value of 1. 0, and 0.8, respectively. In the third sample $D5^{(3)}$, $x=1$, $x=2$, and $x=3$ have values of 1, 0.7, and 0.6, respectively. The emission wavelengths for all three compositions of QD are plotted in Fig. 8(b). The grading of the QD/buffer interface produces only a small blue shift in the emission spectrum. The larger the interface gradient, the larger the blue shift. A maximum blue shift of 47 nm ($D5^{(2)}$ at $x = 0.45$) and 70 nm ($D5^{(3)}$ at $x = 0.45$) is observed. The results give a quantitative measure of the interface effects on the emission spectra and indicate that the interface details are not of utmost criticality in this particular system.

### D. QD Size Variation Effect

Experimentally, it is very hard to create a QD of precise size or measure the exact QD size after capping. Modeling such devices should therefore also consider the effects of size
fluctuations. To quantify the effect of the QD size on the wavelength of emission spectra, we simulated two different size variations of $D5$ (base diameter 20 nm, height 5 nm). Fig. 8(c) shows the emission wavelength as a function of In fraction ($x$) of the SRCL for: 1) base diameter $= 21$ nm and height $= 5$ nm and 2) base diameter $= 20$ nm and height $= 5.5$ nm against $D5$. In both cases, the emission spectra wavelengths shift toward higher values (redshift). Average redshifts of $\sim 40$ and $\sim 120$ nm are calculated for cases 1) and 2), respectively. Fig. 8(c) compares our results with the experimental data [6] (dotted lines). The three dotted lines are for the same InGaAs compositions grown by low-pressure metalorganic chemical vapour deposition (MOCVD) using trimethylindium (TMI), triethylgallium (TEG), and tertiarybutylarsine (TBA) as the source materials at the total pressure of 76 torr. Three samples of the same QDs were grown by changing the growth conditions of InAs QDs and the source materials of the GaAs capping layer. The conditions of the TBA partial pressure, the growth rate of InAs QDs and the source materials of GaAs capping layer are shown in [6, Table I]. The comparison of our results with these experimentally reported curves ([4, Fig. 4]) show that a QD with base diameter 21 nm and height 5 nm matches the experimental curve more closely. Hence, we conclude that the QD in the experiment might have a height of 5 nm and base diameter of around 21 nm.

E. Change in Electronic Confinement

The earlier sections showed that the SRCL strongly modifies the strain profiles. Stepping back, one notices that a material is introduced that effectively reduces the electronic confinement, since the InGaAs bandgap is smaller than the GaAs confinement buffer bandgap. One could argue [8] that this reduction in confinement is the reason for a reduced bandgap since the wave functions can leak out from the QD. Here, we test this argument by inserting a strain reducing buffer that has virtually the same strain effects as InGaAs, but a larger gap. We introduce an $In_xAl_{1-x}As$ SRCL for $x = 0.12$ and $x = 0.4$ in $D5$. Everything else is kept unchanged. The change in the optical gap is found to be only 14 meV (for $x = 0.12$) and 13.4 meV (for $x = 0.4$) shown as stars in Fig. 8(a). Since the $In_xAl_{1-x}As$ SRCL has a larger gap (by 1.3 eV) as compared to the $In_yGa_{1-y}As$, a small change in the optical gap indicates that the reduced barrier height on the top side of the QD has only a minor contribution in the significant observed redshift. This is because the electron and the hole states are strongly localized within the band edge diagram wells (see Fig. 4 and, for 3-D volume representations, Fig. 9). In fact, especially for the holes, it can be observed that the strain confines the wave function more tightly into the quantum well. This effect is also observed in experiment [10]. A slight clockwise rotation is found for the excited states $e2$ and $e3$ with an increased In fraction. This rotation can be explained in terms of the hydrostatic stress relaxation at the top of the InAs QD. The negative gradient in the hydrostatic strain causes an unequal stress in the zinc blende lattice structure along the depth, breaking the equivalence of the [110] and the [110] directions. This breaks the degeneracy of the first excited state, called a $p$-state, aligning the $e2$ state in the [110] direction and the $e3$ state in the [110] direction [24, 29]. The reduction of the hydrostatic strain in the growth direction and the shift of the peak of the hydrostatic strain from the top of the dot toward the center of the dot, as evident from Fig. 3, causes this slight rotation in the wave functions of the $e2$ and the $e3$ states.

F. Wave Function Confinement and Symmetries

Fig. 9 plots the calculated first four electron ($e1$, $e2$, $e3$, and $e4$) and the first two hole ($h1$ and $h2$) wave function squared for $x = 0$, 0.18, and 0.4 in $D5$, $x = 0.4$ in $D10$, and 5-nm-thick $In_{0.4}Al_{0.6}As$ SRCL (last row). The green region shows the boundaries of the InAs QD. The blue and the red colors show the intensity of magnitude (blue is lowest and red is highest).

G. Neglected Physical Effects

Although the tight binding approach and NEMO 3-D can indeed treat excitonic effects [37] and piezoelectric effects [14],
[15], [24], we neglect these effects in this paper. Excitonic effects lower the bandgap by a typical value of 10–30 meV corresponding to a change of ∼15–47 µm, which is negligible in comparison to the overall experimental uncertainty, as demonstrated by the fluctuations due to interface interdiffusion/softness and QD size uncertainty. The piezoelectric effects have importance in the ordering and energy splitting of the excited states and are of order 5 meV [24]. Since we are not critically interested here in the polarization of the emitted or absorbed light from excited states, we also neglect this effect.

H. Nano-TCAD Deployment on nanoHUB.org

NEMO 3-D was originally developed at the National Aeronautics and Space Administration (NASA) Jet Propulsion Laboratory from 1998 to 2003. It continues to be developed at Purdue University with algorithmic and physics refinements. In September 2005, an educational version of NEMO 3-D was released on nanoHUB.org that allows the computation of particle in a box states for various geometries, their intraband transitions, and the visualization of 3-D volume rendered wave functions (see sample screen shots in Fig. 10). The computation happens extremely rapidly since the educational version only contains the single “s” orbital model, which corresponds to an effective mass model. The growth and use of the tool on nanoHUB.org has been strong (Fig. 10, inset). Over 1660 users have run over 15 500 simulations since the release of the “Quantum Dot Lab.” Stabilization of grid computing resources now allows us to deploy the full NEMO 3-D version that requires about 10 h on 60 CPUs for the problem sizes presented here.

IV. CONCLUSION

A detailed qualitative and quantitative analysis of the strain relaxation, the QD volume, the AR changes, and the reduction of the barrier height on the SCRL side was presented. The hydrostatic and the biaxial strain relaxations in the growth direction change the electron and hole confinement potentials and contribute to the redshift of the emission spectra. The volume and the AR of the QD increase as the In concentration of the SCRL increases. For large values of the In fraction in InxGa1−xAs (above 0.2), the increased AR becomes a significant source of the energy shift in the strain-reduced QDs. The SRCL-induced barrier height reduction, buffering the InAs QD, has only a negligible effect in the overall energy shift, as shown by an InAlAs comparison. The QD boundary and the surrounding buffer interface softness cause a small blue shift in the emission spectra. A brief size variation study points to a slightly larger base width than reported experimentally. Both the interface softness study and the size variation study show that the physical processes presented here are robust against experimentally unavoidable imperfections. The NEMO 3-D tight binding model achieves an astonishing agreement with experimental data reproducing the nonlinear change in the optical bandgap with the introduction of an SRCL. No parameter [16] adjustment was done for this multimillion-atom electronic calculation. The close quantitative agreement of our theoretical analysis with experimental evidence [6] enables us to gain significant insight into the physics of this system. Continuum strain and electronic structure theories, such as an effective mass model or a k·p method, which do not account for the atomistic details, cannot achieve such detailed explanation or might even lead to incorrect conclusions.

APPENDIX A

The effects of a change in the QD AR can be estimated through a very simple effective mass model. Starting from a simple particle in a box model

\[ E_{n,x,n,y,n,z} = \frac{\hbar^2}{2m_e} \left( \frac{n_x^2}{D_x^2} + \frac{n_y^2}{D_y^2} + \frac{n_z^2}{D_z^2} \right) \]

where, \( D \) is the diameter and \( H \) is the height of the box.

For the ground state energy, \( n_x = n_y = n_z = 1 \)

\[ E_0 = \frac{\hbar^2}{2m_e} \left( \frac{2}{H^2} + 1 \right) \]

Now, the relative variation of the ground state energy as a function of \( D \) and \( H \) is

\[ \frac{\Delta E_0}{\Delta D} = \frac{\Delta E_0}{\Delta H} (0.5 AR^{-3}) \]

\[ AR = \frac{H}{D} \]

Hence, for the low-AR QDs (AR < 0.3), the variation of ground state energy is much more sensitive to height than to the diameter [22].

The quantitative effect of the AR change depicted in Fig. 5 can be estimated with this simple model as follows:

- \( m^* \) for electron = 0.023 \( m_o \), \( m^* \) for holes = 0.41 \( m_o \), \( m_o = 9.1 e - 31 \text{ kg} \) (masses taken from [32])
- \( h = 6.626 e - 34 \text{ J/s} \), \( E_{gap} \) of InAs = 0.354 eV (neglecting strain effects).

Now, using (4)

for \( D = 22.15 \text{ nm and } H = 5.43 \text{ nm} \)

- optical bandgap = \( E_0 \) (electron) + \( E_0 \) (hole) + 0.354 \( \sim 1.01 \text{ eV} \).

For \( D = 22.026 \text{ nm and } H = 5.69 \text{ nm} \)

- optical bandgap = \( E_0 \) (electron) + \( E_0 \) (hole) + 0.354 \( \sim 0.95 \text{ eV} \).
Hence

\[ \text{change in optical gap} = 1.01 - 0.95 = \sim 60 \text{ meV}. \]

Hence, with the simple effective mass model and the changes in QD shape from Fig. 5, the effect of QD shape change is estimated to be 60 meV. This is comparable to the analytical estimate of 88 meV bandgap reduction due to strain alone. This simple effective mass model does not appropriately account for the effects of nonparabolicity. Also, the effects of strain deformation are not included. Appendix C presents a simple numerical model that includes these effects.

**APPENDIX B**

To calculate the contribution of AR variations alone, the electronic structure of a freestanding dome and box-shaped InAs QD (without any surrounding GaAs buffer) is computed using NEMO 3-D. The strain calculations are turned off to exclude the strain contribution. The optical bandgap is computed from the ground electron and hole energy levels. The following cases of InAs QD dimensions, taken from Fig. 5 (inset), are simulated separately.

**Case 1:** Diameter = 22.018 nm, height = 5.5 nm \( \Rightarrow \) the optical bandgap is 1.03 eV for the dome and 0.43 eV for the box shape.

**Case 2:** Diameter = 22.150 nm, height = 5.5 nm \( \Rightarrow \) the optical bandgap is 1.0399 eV for the dome and 0.431 eV for the box shape.

**Case 3:** Diameter = 22.018 nm, height = 5.69 nm \( \Rightarrow \) the optical bandgap is 0.931 eV for the dome and 0.397 eV for the box shape.

Hence, we find that the reduction in the base diameter results in approximately blue shifts of 1.03 – 1.03 = \sim 10 meV for the dome shape, and \sim 1 meV for the box shape and the increase in the height results in about 1.03 – 0.931 = \sim 100 and \sim 33 meV redshift of the emission spectra, respectively. Compared to the simple effective mass model in Appendix A, we include the effects of nonparabolocity, and band coupling accounts for about 27 meV blue shift and QD dome shape about 67 meV redshift.

**APPENDIX C**

Appendix A estimates the effect of AR from a simple effective mass model with parabolic band assumption. InAs is known to be a very nonparabolic material. In this appendix, we estimate the effects of nonparabolocity of InAs bands, strain, and AR through the following simple numerical experiment.

1) From a single bulk InAs unit cell (with and without strain), we compute the bulk \( E(k) \) dispersion.
2) Now, assuming a rectangular, infinite wall QD, we quantize the momentum vector \( k \) in \( x-, y-, \) and \( z-\)directions.
3) Extract the bandgap and the local effective masses in the vicinity of the quantized \( (k_x, k_y, k_z) \) tuple on \( E(k) \) diagram.
4) By varying \( (k_x, k_y, k_z) \) according to AR variations, we can estimate its effect.

5) From the strain distortions of the InAs cell, we can explore the effect of strain. The procedure is as described as follows. The basic \( E-k \) dispersion relation is

\[ E_{k_x,k_y,k_z} = \frac{\hbar^2}{2\pi^2} \left( \frac{k_x^2}{m_x^*} + \frac{k_y^2}{m_y^*} + \frac{k_z^2}{m_z^*} \right) \]  

where \( k_x = \pi/L_x, \ k_y = \pi/L_y, \ k_z = \pi/L_z, \) and \( L_x, L_y, \) and \( L_z \) are dimensions in \( x-, y-, \) and \( z-\)directions, respectively. Correct effective masses in \( x-, y-, \) and \( z-\)directions at the point of dispersion \( (k_x, k_y, k_z) \) are calculated from the band structures of InAs in \( x-, y-, \) and \( z-\)directions, respectively. The point of dispersion \( (k_x, k_y, k_z) \) is computed from dimensions of InAs QD taken from Fig. 5. Fig. 11 shows two sample cases. The correct effective masses and corresponding optical gaps computed from (7) are given in Table II. Using correct effective masses from Table II, we conclude that

\[ \text{AR contribution} = 0.56 - 0.482 = \sim 78 \text{ meV} \]

\[ \text{AR + strain contribution} = 0.831 - 0.687 = \sim 144 \text{ meV} \]

\[ \text{strain contribution} = 144 - 78 = \sim 66 \text{ meV}. \]

We also computed the bandgaps directly from \( E(k) \) diagram instead of using (7). This is done by plotting \( E(k) \) diagram in [1 1 1] direction and looking at the point of dispersion.
These numerically computed bandgap variations are

\[
\text{AR contribution} = \sim 72 \text{ meV}
\]

\[
\text{AR + strain contribution} = \sim 132 \text{ meV}
\]

strain contribution = 132 – 72 = \sim 60 \text{ meV}.

These results from simple analytical expressions with correct effective masses show a close qualitative match with our simulation result and provide a qualitative validation of our simulator. Also, \sim 12 \text{ meV} difference between AR contribution calculated in Appendixes A and C highlights the importance of using correct effective masses, taking into account the nonparabolicity of the bands.

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