Supporting Information for:

Highly-Strained III-V-V Co-Axial Nanowire Quantum Wells with Strong Carrier Confinement

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S1: Schematic of AlGaAs/GaAs and GaAsP/GaAs nanowire quantum wells

![Schematic Diagram](image-url)
Figure S1. Band structure and carrier dynamics schematic of NW QWs composed of (a) AlGaAs and (b) GaAsP material systems.

As can be seen in Figure S1a, the AlGaAs/GaAs quantum well (QW) is built on a GaAs core nanowire (NW). The GaAs core forms a potential minimum and can therefore trap a large number of carriers at the centre of the NW. As a result, these carriers cannot contribute to the quantum well emission. In contrast, the GaAsP/GaAs QW is built on a GaAsP core NW and there is no potential minimum at the centre of the NW (Figure S1b). A higher fraction of injected carriers are hence captured by the quantum well and contribute to its emission.

S2: Crystalline properties of a single quantum well NW.

![Figure S2. Low magnification bright field scanning transmission electron microscopy (BF-STEM) image showing the bottom, middle and tip of the GaAsP NW containing one GaAs quantum well. The yellow arrow in (c) points to one threading dislocation.](image)

As shown in Figure S2a, the bottom of the NW has a uniform contrast and no stacking-fault related contrast difference is observed, indicating a high-quality, single crystal structure. The middle part has a slight contrast difference (Figure S2b), which indicates the generation of stacking faults. The tip has an irregular morphology which accompanies a higher-density of stacking faults and threading dislocations (Figure S2c).^1

S3: Dislocation analysis of the GaAsP-GaAs interfaces and strain distribution in the multiple QWs
Figure S3 (a) Low-resolution TEM image of one NW with a single GaAs-GaAsP QW. (b), (d), (f), (h) show high-resolution images of the side-view of the QW interfaces recorded for
different positions along the NW as indicated in (a). These images are for the $<110>$ zone axis. (c), (e), (g), (i) are the corresponding FFT filtered images.

Figure S4 (a) Low-resolution TEM image of the cross section of one NW with a single GaAs-
GaAsP QW. (b) Strain mapping around the QW region. (c), (d), (e) and (f), (g), (h) are high-resolution TEM images and corresponding FFT filtered images for the regions indicated in (a).

Core-shell NW heterostructures may form line and/or loop type dislocations due to lattice mismatch.\textsuperscript{2,3} Figure S3b, d, f and h show high-resolution images of the QW interfaces for different positions along the nanowire length. No strain induced dislocations are observed. This is further confirmed by the fast Fourier transform (FFT) filtered images shown in Figure S3c, e, g and I, which highlight the \{111\} lattice planes. Despite the presence of planar defects (close to the tip), and slightly varying core and QW thicknesses, no loop type dislocations (which should be visible as extra planes within the GaAsP shells) are seen along the length of the NW. For the NW cross-section, strain information in the QW region is shown in Figure S4b. No misfit dislocations are observed in the region of the QW interfaces.\textsuperscript{4} This is also confirmed by the high-resolution TEM images and corresponding FFT filtered images shown in Figure S4c-h.

**S4: Calculation of QW electron and hole confinement energies.**

![Graph](image)

**Figure S5.** Dependence on QW width of the emission wavelength and activation energies for electrons and holes.
We have modelled energy band edge profiles and calculated the lowest confined electron and heavy-hole energies using NextNano software. This uses an 8-band k.p envelope function approximation to solve the Schrödinger equation for the single GaAs-GaAsP NW QW structure in one dimension along a line joining two opposite NW facets. The simulation includes pseudomorphic strain, with the 46% phosphorous outer shells assumed to be unstrained as these represent the largest volume of material. The calculated QW emission wavelength as a function of QW width is shown in Figure S5 (black curve), and the electron and hole activation energies (the difference between the QW confined states and relevant barrier band edge) are shown in blue and red, respectively. The experimentally measured QW PL emission varies between ~730-740 nm, indicating a QW width between ~6.5 and 9 nm. For a width of 8 nm the activation energies for electrons and holes are calculated to be 115 and 300 meV, respectively (Figure S5). The former value is close to the activation energy determined from the temperature dependent PL (Figure S7), indicating that electron loss from the QW is the dominant factor in the quenching of the PL.

**S5: Lifetime dynamics of the QW carriers.**

![Figure S6](image)

**Figure S6.** (a) PL spectrum and (b) decay transients for different detection energies (emission wavelengths) measured from the stacking-fault-free segment of a single QW NW for a sample temperature of 6K.
The lifetimes of the QW confined carriers were measured for a range of energies across the PL emission (Figure S6a) and for a sample temperature of 6K. Figure S6b shows typical PL transients. The lifetime is longer for carriers with a lower energy (longer emission wavelength) and exhibits an initial plateau-like behaviour consistent with the transfer of carriers from high to low energy states within the QW.

S6: Temperature dependence of the photoluminescence

The temperature dependence of the photoluminescence (PL) intensity was measured for an ensemble of NWs. The integrated intensity, normalised to the low temperature value, is shown in Figure S7. The temperature-dependent PL quenching processes can be analyzed by fitting the data using a modified Arrhenius equation,\(^6\)

\[
I(T) = \frac{I_0}{[1 + A_1 \exp(-E_1/kT) + A_2 \exp(-E_2/kT)]}
\]

where \(I_0\) is the low temperature intensity, \(E_1\) and \(E_2\) are activation energies for processes that remove carriers from the optically active state, the QW in this case, and \(A_1\) and \(A_2\) characterize the strengths of the two processes and are determined in part, by the number of states to which carrier loss can occur. The fitting procedure gives a value for \(E_1\) of 15±1 meV; this process is associated with non-radiative recombination centres at

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**Figure S7.** Arrhenius fitting of temperature-dependent PL data.
the GaAsP surface. \(^6\) \(E_2\) is 125\(\pm\)12 meV.

The ratio \(A_1/A_2\) for the current structure (8\(\times\)10\(^{-4}\)) is much smaller than previously reported values for related structures, for example 2\(\times\)10\(^{-2}\) for a GaAs/GaAs\(_{0.85}\)P\(_{0.15}\) coaxial structure without a QW\(^6\) and infinity for pure GaAs NWs. This result suggests that carrier loss to surface non-radiative recombination is greatly reduced in the present structure. For example, carriers on the inner side of the QW are inhibited from reaching the surface due to the deep QW.

**S7: Significantly enhanced PL emission via the addition of a QW**

![Figure S8](image)

**Figure S8.** (a) Comparison of 10K PL spectra from an ensemble of NWs, with comparable NW morphology and density. The excitation laser power was 40 mW. Red: GaAsP/GaAs QW NWs, blue: GaAsP NWs without a QW and without surface passivation, and pink: GaAsP NWs without a QW but with surface passivation. (b) Integrated PL intensity of the three different NW samples as a function of laser excitation power.

The influence of the QW on the PL emission of the NW is further studied by comparing the optical properties of core-shell GaAsP NWs grown with and without a GaAs QW. Figure S8a shows 10K macro-PL spectra recorded from ensembles of the as-grown NWs which, for the GaAsP/GaAs NW QWs, probe both the defect-free lower and defective tip regions. The spectrum of the NW QW sample comprises two peaks, representing emission from the defective tip at \(\sim\)765nm and from the defect-free region.
at ~740nm. Due to the high carrier collection efficiency and the strong confinement by the QW, the peak (integrated) intensity of the QW emission for the GaAsP/GaAs NW QW structure is 150 (50) times as intense as that of the reference GaAsP NWs without a QW but with a comparable morphology and density. This enhancement is achieved despite approximately 1/3 of the length of the NW QW sample containing defects. Even with the addition of an InGaP surface passivation layer to a GaAsP NW without a QW, the peak (integrated) intensity of the QW emission remains 20 (10) times stronger. Furthermore, the FWHM of the QW emission (16.2 nm) is significantly narrower than that of the NWs without a QW (37~43nm). Unlike the emission of the pure NWs, the PL from the GaAsP/GaAs NW QW structure varies approximately linearly with increasing laser power over a wide power range, as shown in Figure S8b. In contrast, for the pure NWs the PL appears to saturate at high powers and is always significantly weaker than that of the NW QW. This further confirms the significant improvement in optical quality obtained by adding a QW to the NW structure.

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