Supporting Information For:

Facet-Selective Epitaxy of Compound Semiconductors on Faceted Silicon Nanowires

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Materials and Methods

Faceted Si nanowires (NWs) with diameters from 200 to 400 nm were grown according to a previously described procedure by depositing different thickness Si shells on ca. 100 nm diameter Si NW cores at 775-860 ^{o}C.[1] The growth substrate with the faceted Si NWs was dipped in buffered hydrofluoric acid (BHF; 5173-03; J.T. Baker) for 20 s to remove surface oxide, rinsed for 5 s in deionized water, and then submerged in liquid nitrogen to freeze remaining water on the NW/substrate chip; this process prevents collapse of the low-density NWs via capillary forces during liquid water evaporation.[1] The frozen growth substrate was quickly transferred to the second zone of a 3-zone furnace and the furnace was evacuated to a base pressure of 50 mTorr, as previously described.[2] Once at base pressure, the furnace was purged three times each with Ar (semiconductor grade; Matheson Tri-Gas; 99.999%) and H_2 (ultrahigh purity; Airgas; 99.999%) and the pressure was set at ~2.8 Torr with a flow rate of 20 sccm H_2. The 3-zone furnace is equipped with a quartz boat with adjustable position using a quartz transfer rod. Prior to the above evacuation and purge, the quartz transfer boat was loaded with either CdS powder (-325 mesh; Alfa Aesar; 99.999%) or milled InP powder (Alfa Aesar; 99.9999%). Once the temperature of zone 1 stabilized at 670-710°C, the quartz rod was used to position the precursor in the center of zone 1. CdS or InP shells were grown on the Si NWs in zone 2 at 450-550°C for 5-40 minutes.

NWs were imaged directly on the growth substrate using a Zeiss Ultra Plus field emission scanning electron microscope (SEM). For plan-view transmission electron microscope (TEM) or scanning TEM (STEM) imaging, NWs were mechanically transferred from the growth substrate to amorphous-carbon coated copper TEM grids (Ted Pella). Cross-sections were prepared by deposition of a protective carbon layer and subsequent lift-out using a Zeiss NVision 40 dual-beam SEM/focused ion beam (FIB) equipped with an Omniprobe micromanipulator. Both the plan-view and cross section NW samples were characterized using an aberration-corrected Zeiss Libra MC TEM operating at 200 keV. STEM-based energy dispersive x-ray spectroscopy (EDS) elemental mapping characterization was completed using an aberration-corrected Hitachi HD-2700 STEM operating at 200 keV.

Photoluminescence images were recorded at room temperature using a scanning confocal microscope (FluoView FV1000; Olympus America Inc.) with 473 nm excitation and a 490-540

nm band pass filter to pass photoluminescence and block excitation laser light. Optical spectroscopy at room temperature utilized a home-built epifluorescence microscope.[3] A continuous-wave 405 nm diode laser (LaserGlow Technologies) was collimated and focused to a ~1 μm diameter spot with incident power ~900 μW using a 40x objective lens (NA = 0.75; Olympus America Inc.). The laser and luminescence were passed through a 405 nm dichroic and subsequently through two 450 nm long pass filters to remove excitation light and finally to a 150 mm spectrometer (SP150; Princeton Instruments; 300 lines mm^{-1} grating) equipped with a CCD detector (NTE 2; Roper Scientific).

Supplementary Figures

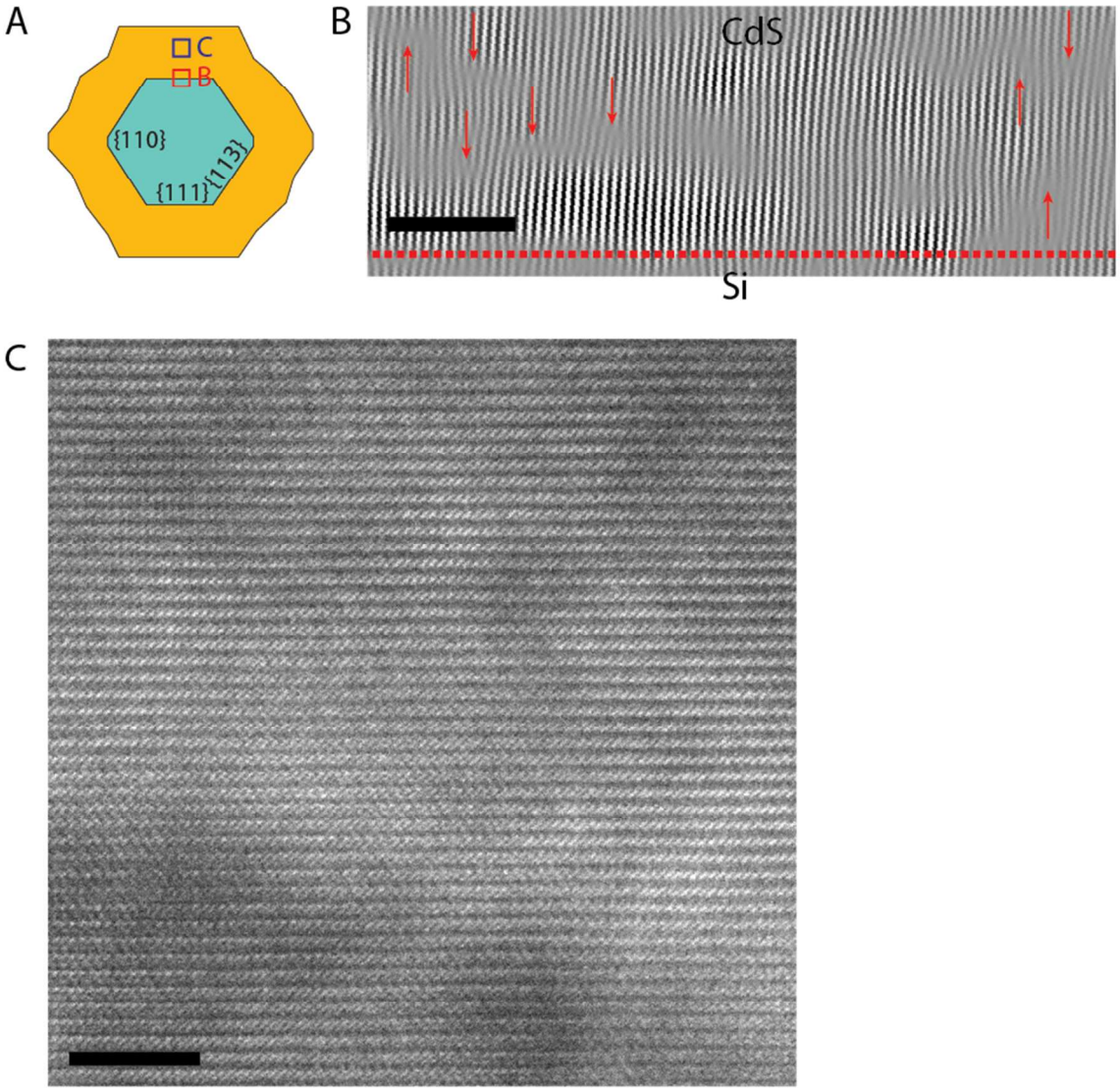

Figure S1. Additional characterization of the Si-CdS heterostructure NWs. (A) Schematic depicting the locations from which the cross-sectional TEM images in (B) and (C) were recorded. (B) Fourier-filtered TEM image of the region of the Si-CdS {111} interface shown in Figure 3B derived from the CdS<0110> reflection. Scale bar, 5 nm. The image reveals misfit dislocations (red arrows) ~4 nm from the Si-CdS interface (dashed red line). (C) Cross-sectional TEM image of the CdS grown on the {111} facet of a Si NW ~100 nm from the Si-CdS {111} interface. Scale bar, 5 nm. The TEM image reveals that the CdS in this region is practically free of defects, suggesting that despite the initial formation of misfit dislocations near the interface, the majority of the CdS has high crystalline quality.

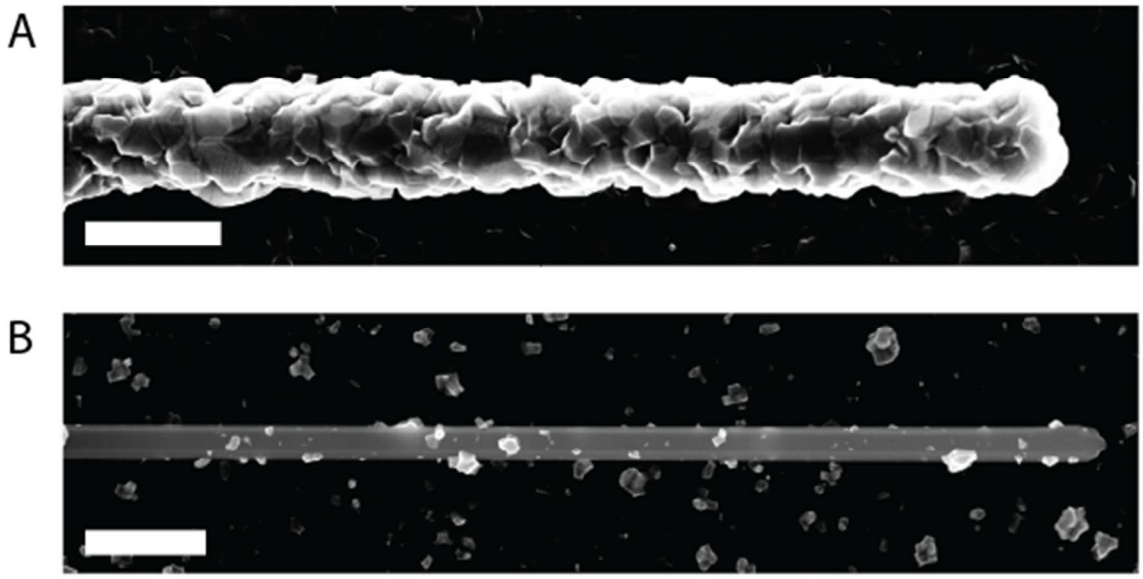

Figure S2. CdS growth on faceted Si NWs without removing the Si native oxide prior to growth. SEM images of (A) upstream and (B) downstream Si/CdS heterostructure NWs grown without a BHF etch prior to CdS deposition. Upstream, the CdS deposits conformally on the NWs but lacks the well-developed surface facet seen in the NWs grown with BHF etch prior to CdS deposition as in Figure 3; downstream, no continuous CdS shells deposit on the Si NWs, in contrast to those shown in Figure 1. Scale bars, 1 μm.

Supplementary References

1. Kempa, T. J.; Cahoon, J. F.; Kim, S-K.; Day, R. W.; Bell, D. C.; Park, H-G.; Lieber, C. M. *Proc. Natl. Acad. Sci. USA* **2012**, 109, 1407–1412.
2. Jiang, X.; Xiong, Q.; Nam, S.; Qian, F.; Li, Y.; Lieber, C. M. *Nano Lett*., **2007**, 7, 3214–3218.
3. Agarwal, R.; Barrelet, C. J.; Lieber, C. M. *Nano Lett.* **2005**, 5, 917–920.