Supporting Information

Hole gas accumulation in p-Si/i-Ge core-shell and p-Si/i-Ge/p-Si core-

double shell nanowires

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1. Structural characterization of p-Si/i-Ge core-shell NWs

The dimensions of p-Si/i-Ge core-shell NWs were measured from SEM images. To get a clearer understanding of the NW appearance, SEM images of p-Si/i-Ge core-shell NWs with various i-Ge shell growth times of 15, 30, 60, and 90 seconds on core p-Si NWs doped with 0, 0.1, 0.2 and 0.5 sccm B_2H_6 gas flux were imaged as shown in Figure S1. The diameter of the NWs increased with gas flux and shell growth time as summarized in Figure S1 (e).





Figure S1. (a)-(d) SEM images of p-Si/i-Ge core-shell NWs with varying B doping concentrations and shell growth time conditions. B_2H_6 gas flux was varied from 0 sccm to 0.5 sccm and shell growth time was varied from 15 sec to 90 sec. The cale bar for all images is 5 μ m. (e) The diameter of p-Si/i-Ge core-shell NWs as a function of shell growth time.

The interface of p-Si/i-Ge core-shell NWs is highly crystalline and free of defects as shown in Figure 2. More detailed high resolution TEM images are shown in Figure S1. In Figures S2 (a) and (b), the i-Ge shell layers can be clearly distinguished from the p-Si core NWs. The high resolution TEM images in Figures S1 (c) and (d) showed clear lattice fringes, which demonstrate that the p-Si/i-Ge core-shell NWs are single crystalline. No defects at the interface between the p-Si core NWs and i-Ge shell layer were observed with a Ge shell thickness below 15 nm.



Figure S2. (a) Low-resolution and (b)-(d) high-resolution TEM images of p-Si/i-Ge core-shell NWs with a B_2H_6 gas flux of 0.1 sccm and shell growth time of 60 sec.

2. B doping effect on the Si and Ge optical phonon peaks

Raman spectroscopy is an important technique for characterizing crystallinity, stress and electrical activation of dopants in p-Si/i-Ge core-shell NWs. The Raman spectra of the core-shell NWs grown with B₂H₆ fluxes of 0.1 sccm and 0.5 sccm are shown in Figure 3. To demonstrate the effect of doping in p-Si/i-Ge core-shell NW structures, more detailed data from nanowires grown with various i-Ge shell growth times of 15, 30, 60, and 90 seconds and various doping concentrations in p-Si core NWs of 0, 0.1, 0.2, and 0.5 sccm are shown in Figure S3. The Si optical phonon peaks decreased with increasing shell growth time, and the opposite behavior was observed for the Ge optical phonon peak as shown in Figures S3 (a)-(d). This is due to the increase Ge shell layer thickness. Asymmetric broadening of the the Si optical phonon peaks increased with increasing doping concentration, which can be attributed to the Fano effect, indicating the electrical activation of B atoms in p-Si core NWs. For the Ge optical phonon peaks, asymmetric broadening towards lower wavenumber with increasing B doping concentration in the p-Si core NW region was also observed. The results could be explained by the Fano effect which is caused by hole gas accumulation in the i-Ge shell region from p-Si core NWs. Moreover, no distinct GeSi alloy optical phonon peak was observed at around 400 cm⁻¹, indicated that the intermixing between Si and Ge and effect of out-diffused B atoms can be ignored under these conditions. Figures S3 (e) and (f) show the dependence of the Si and Ge optical phonon peaks on shell growth time. The B_2H_6 gas flux was kept at 0.2 sccm for both. These results were consistent with those shown in Figures 3 (c) and (d).



Figure S3. Raman spectra of p-Si/i-Ge core-shell NWs with various shell growth times of 15, 30, 60, and 90 seconds. The core p-Si NWs grown with B_2H_6 fluxes of (a) 0, (b) 0.1, (c) 0.2, and (d) 0.5 sccm. (e) Raman shift of the Si and Ge optical phonon peaks as a function of shell growth time with B_2H_6 fluxes of 0.2 sccm.

3. Core-shell nanowire formation induced stress

Figure S4 shows the XRD spectra of p-Si/i-Ge core-shell NWs with a B_2H_6 flux of 0.2 sccm and various shell growth times of 15, 30, 60, and 90 seconds. The Ge (111) peaks shifted to lower angles and Si (111) peaks shifted to high ones with increased shell growth time. These results were consistent with the XRD spectra of p-Si/i-Ge core-shell NWs formed with B_2H_6 fluxes of 0.1 and 0.5 sccm as shown in Figures 4 (a) and (b). The average lattice constants were calculated by fitting the XRD peaks, as shown in Figures 4 (c) and (d).



Figure S4. XRD spectra of the p-Si/i-Ge core-shell NW structure formed by B_2H_6 fluxes of 0.2 sccm and various shell growth times.

4. Crystallization of p-Si core NWs by annealing process

To improve the crystallinity and electrical activation of B dopant atoms in p-Si core NWs, thermal annealing was performed in vacuum prior to the shell deposition. The annealing temperature and time were fixed at 800 °C and 30 min. Figure S5 shows Raman spectra of pSiNWs formed with SiH₄ (19 sccm) and B_2H_6 (0.5 sccm) gas fluxes before and after annealing. The peak intensity of the Si optical phonon peak significantly increased after annealing and asymmetric broadening due to the Fano effect was also observed, showing that thermal annealing is important to improve NW crystallinity and the electrical activation of dopants.



Figure S5. Raman spectra of p-SiNWs formed with a SiH₄ gas flux of 19 sccm and B_2H_6 gas flux of 0.5 sccm. The black and red lines represent as-grown nanowires and samples annealed at 800 °C for 30 min, respectively.