Supplementary Information for "The Effect of Structural and Chemical Bonding Change on Optical Properties of $Si/Si_{1-x}C_x$ Core/Shell Nanowires"

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Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

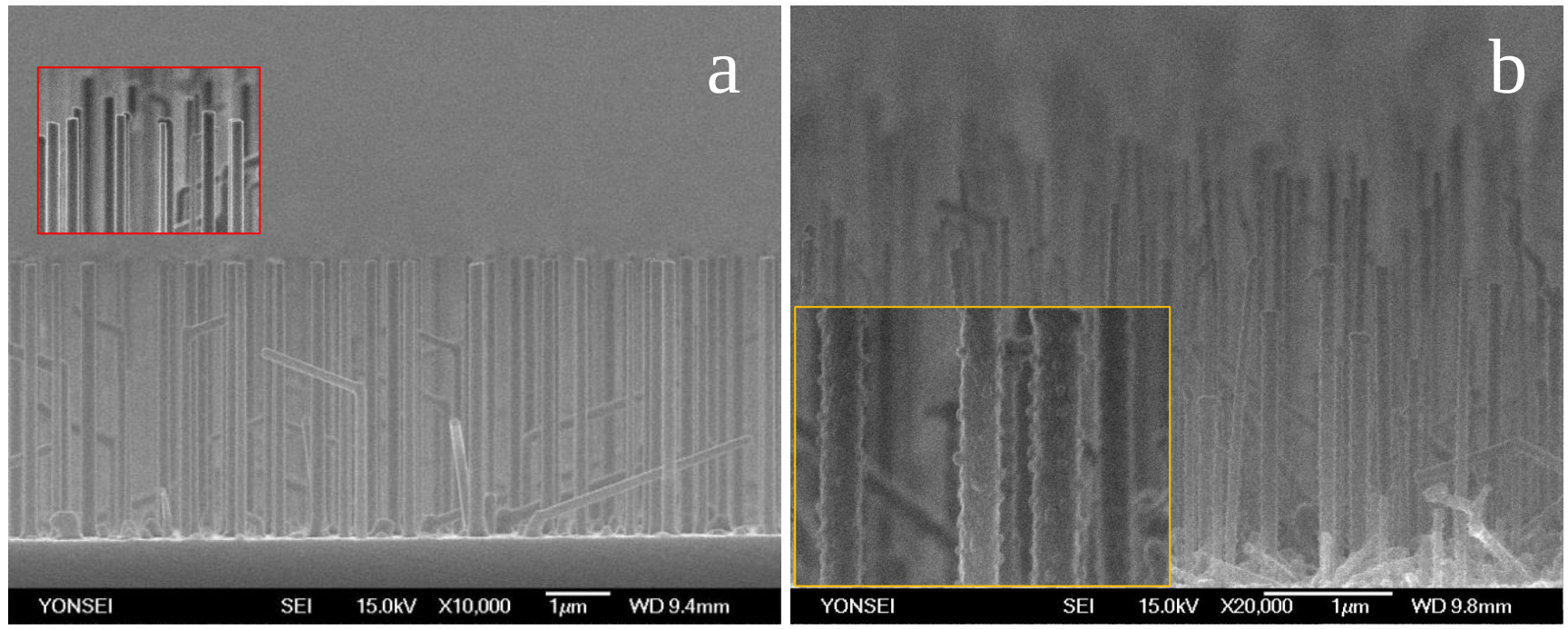


Figure S1. FE-SEM images of the Si/$Si_{1-x}C_x$ core/shell. (a) as-grown Si core NW after the removal of the Au tip at top of the wire, and (b) Si/$Si_{1-x}C_x$ core/shell NWs annealed at 750 ℃ in a vacuum.

Supporting Figure S1. Lee *at. al.*

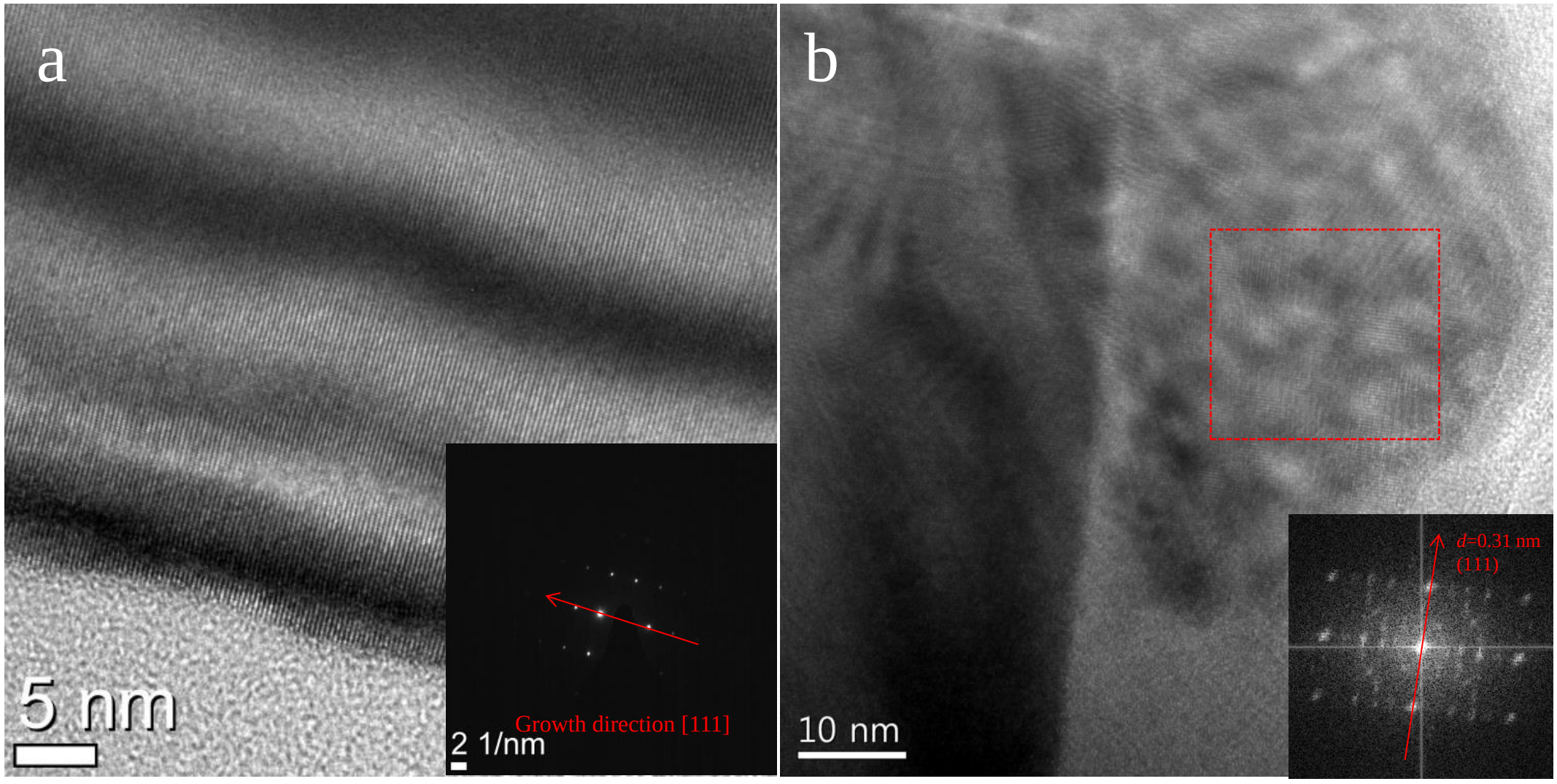


Figure S2. (a) HR-TEM image of as-grown Si core NW after the removal of the Au tip at top of the wire, which presents single crystal structure. (b) HR-TEM image of $Si/Si_{1-x}C_x$ core/shell NWs annealed at 600 ℃ in a vacuum. In this case, $Si_{1-x}C_x$ shell became thick and poly-crystallization.

Supporting Figure S2. Lee *at. al.*

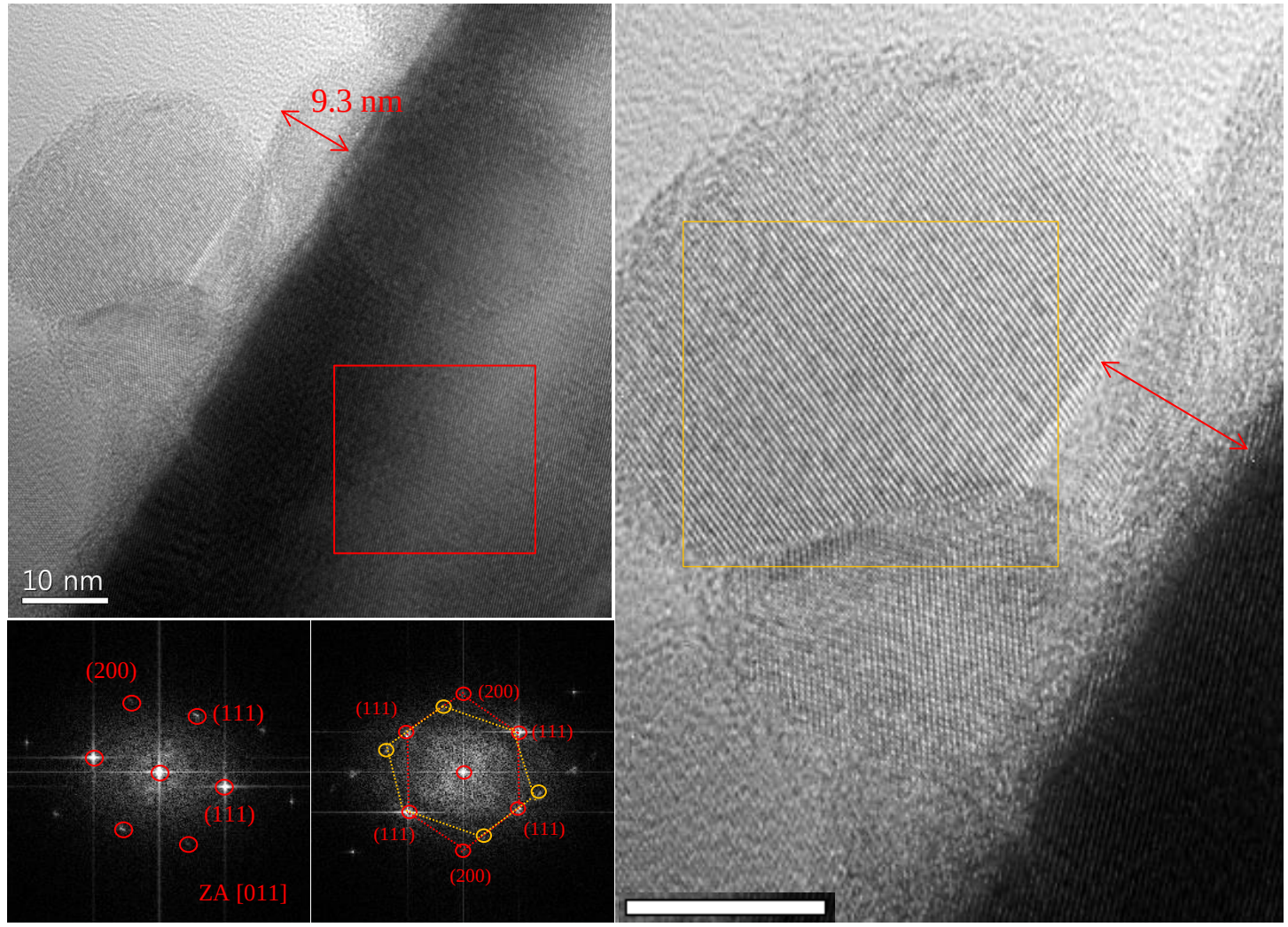


Figure S3. HR-TEM images of the Si/$Si_{1-x}C_x$ core/shell NWs annealed at 750 ℃ in a vacuum. In this case, $Si_{1-x}C_x$ shell was transformed into single crystal structure.

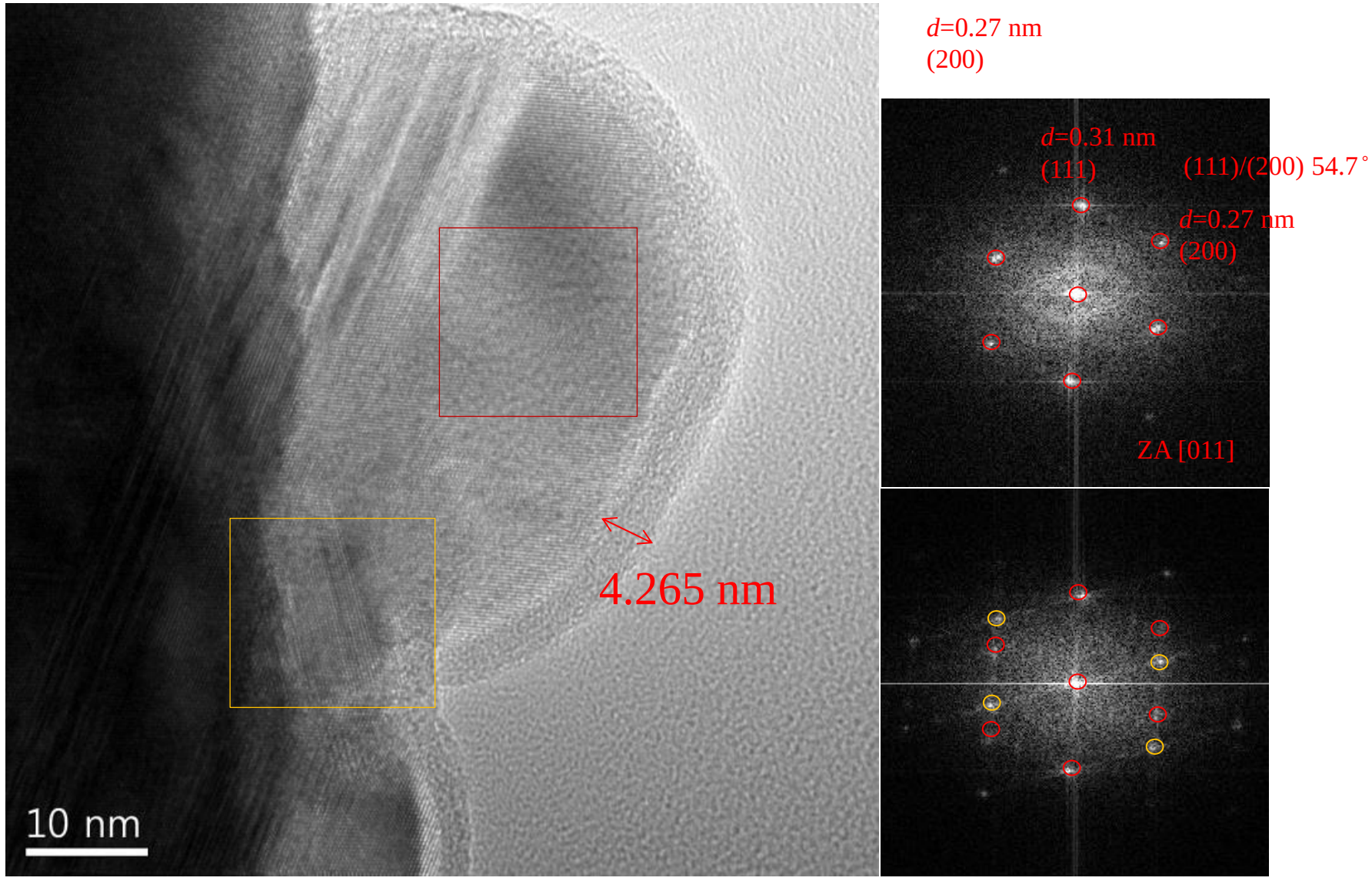


Figure S4. HR-TEM images of the Si/$Si_{1-x}C_x$ core/shell NWs annealed at 750 ℃ in a vacuum. In this case, $Si_{1-x}C_x$ shell was transformed into single crystal structure with an amount of twin defect.

Supporting Figure S4. Lee *at. al.*

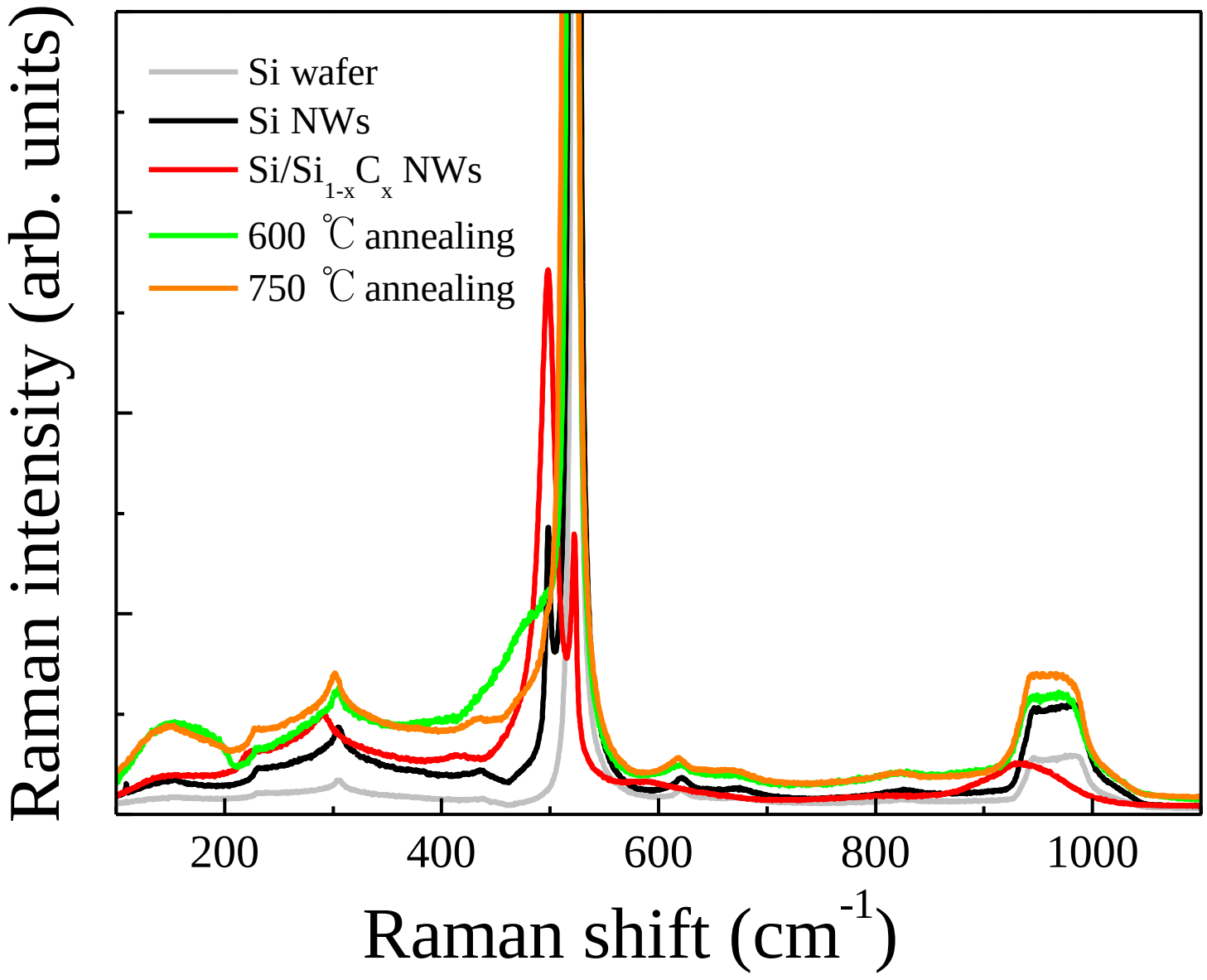
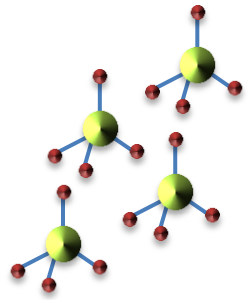


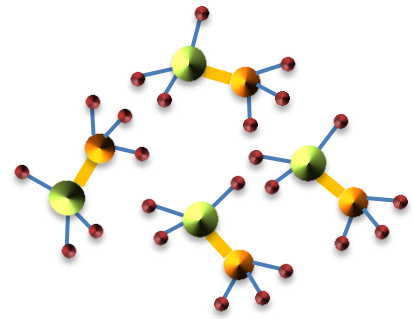
Figure S5. Raman spectra of the $Si/Si_{1-x}C_x$ core/shell NWs as a function of annealing temperature in wide range from 100 ~ 1100 cm^{-1}.

Supporting Figure S5. Lee *at. al.*



SiH_4 gases decomposition

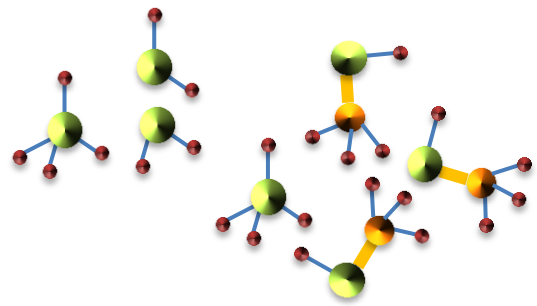
$SiH_4\,(g) \rightarrow SiH_2 + H_2$



SiH_3CH_3 gases decomposition

$CH_3SiH_3\,(g) \rightarrow HSiCH_3$ or $H_2Si{=}CH_2 + H_2$

$Si_{1-x}C_x$ Film Growth



$SiH_2 + CH_3SiH_3\,(g) \xrightarrow{\text{Pyrolysis}} SiH_4\,(g) + SiCH_4$

Figure S6. A schematic diagram of possible decomposition pathways in the gas phase reactions of SiH_4 with CH_3SiH_3 for $Si_{1-x}C_x$ shell growth on Si core NW.

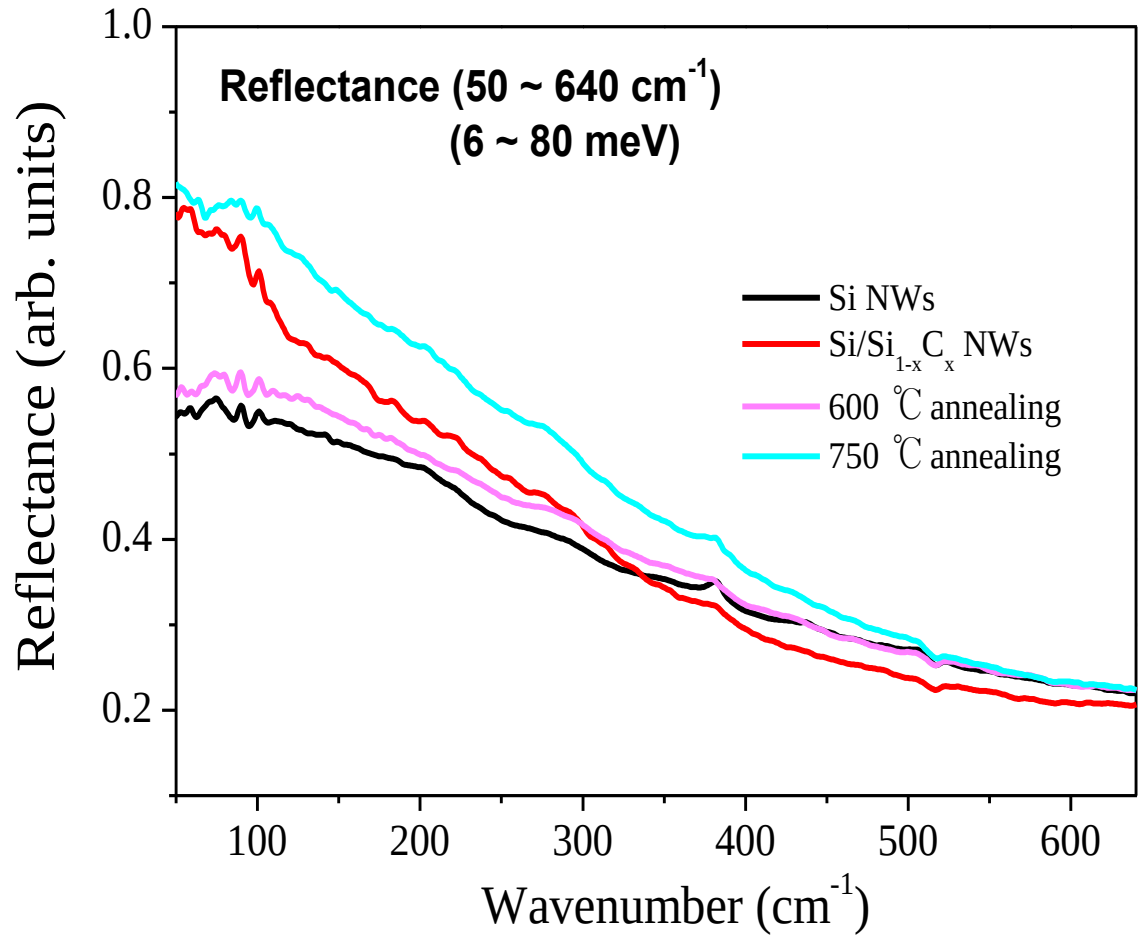


Figure S7. The reflectance spectra in far-infrared region of the $Si/Si_{1-x}C_x$ core/shell NWs as a function of annealing temperature.

Supporting Figure S7. Lee *at. al.*

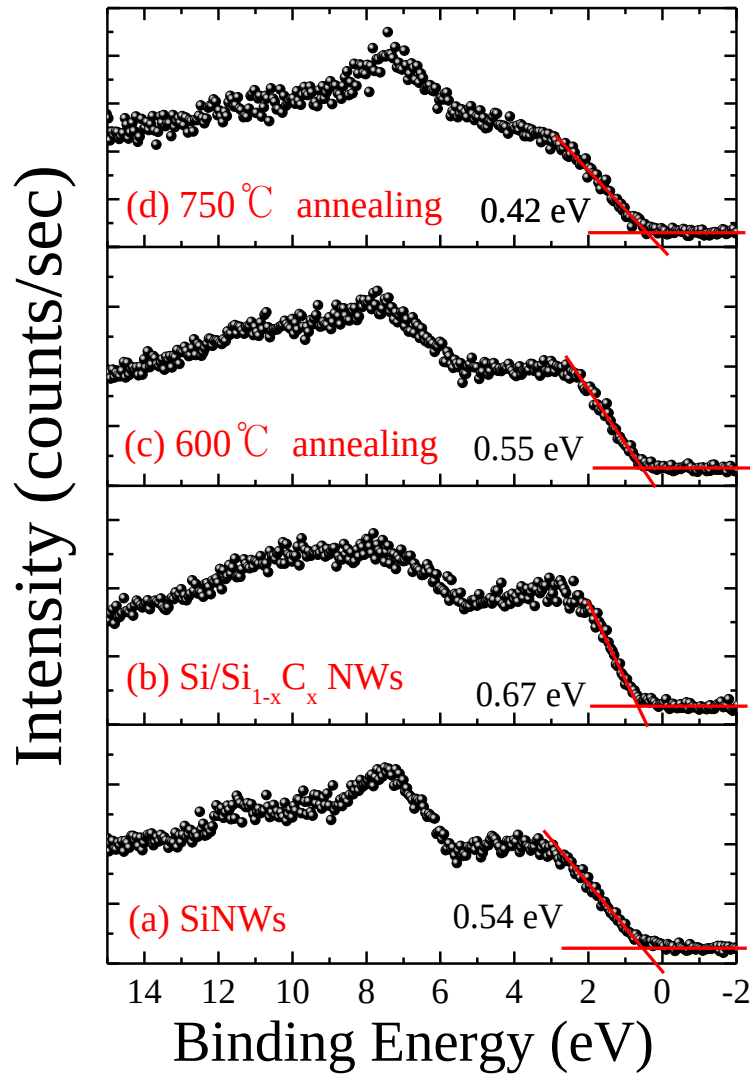


Figure S8. The valence band measured from the $Si/Si_{1-x}C_x$ core/shell NWs as a function of annealing temperature by using XPS.

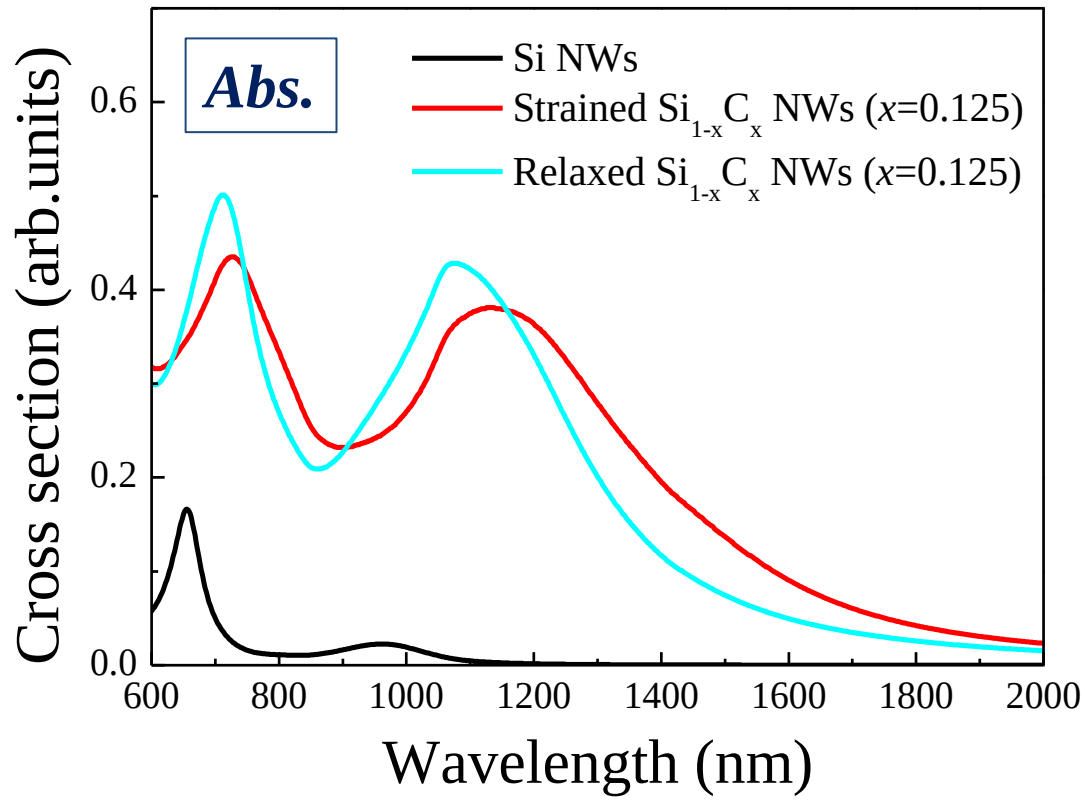


Figure S9. After the irradiation of light source (790 nm), absorption of the Si and $Si_{1-x}C_x$ NW was attained by the result of 2-D FDTD. The $Si_{1-x}C_x$ NW was classified into two kinds; one is strained $Si_{1-x}C_x$ NW including substitutional C atoms randomly distributed in Si lattices and the other is relaxed $Si_{1-x}C_x$ NW consisting of 3nn configuration of C atoms locally existed in Si lattices.

Supporting Figure S9. Lee *at. al.*