Surface Hydrogen Driven Structure Control of Semiconductor Nanowires

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Semiconductor nanowires containing kinking superstructure can serve as an ideal building block for next generation energy conversion device due to their unique transport properties. However, it has remain difficult to fabricate such kinking superstructures, particularly those with long-range structural coherence. Here, we combine high-resolution electron microscopy with operando infrared spectroscopy to show why this is the case for Si nanowires and, in doing so, reveal the interplay between defect propagation and surface chemistry during $(211) \rightarrow (111)$ and $(211) \rightarrow (211)$ kinking. Our experiments show that adsorbed hydrogen atoms are responsible for selecting (211)-oriented growth and indicate that a twin boundary imparts structural coherence. The twin boundary, only continuous at $(211) \rightarrow (211)$ kinks, reduces the symmetry of the trijunction and limits the number of degenerate directions available to the nanowire. These findings constitute a general approach for rationally engineering kinking superstructures and also provide important insight into the role of surface chemical bonding during vapor –liquid-solid synthesis.