

Face-selective tungstate ions drive zinc oxide nanowire growth direction and dopant incorporation

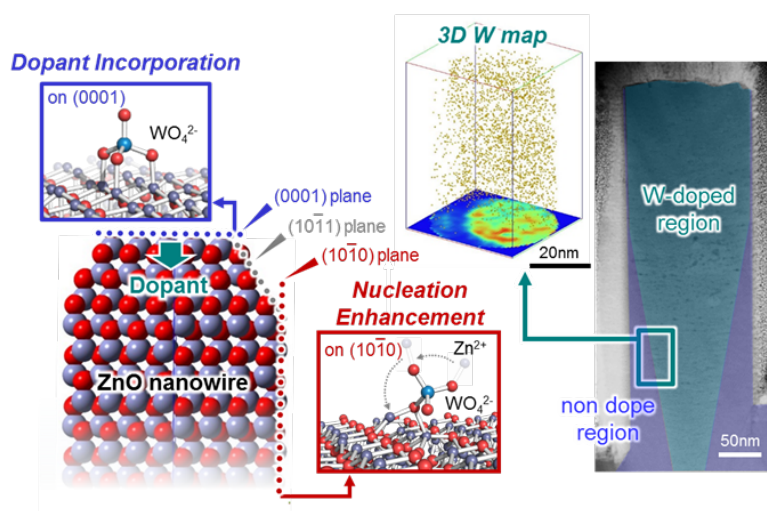
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Tailoring the elemental doping of inorganic nanowires remains an important challenge due to complex dopant incorporation pathways. Here we proposed that the face-selectivity of tungstate ions controls growth direction and dopant incorporation of hydrothermal zinc oxide nanowires. The introduction of tungstate ions on nanowire surface during synthesis unexpectedly enhances nucleation at sidewall $(10\bar{1}0)$ planes, while dopant incorporation occurs only on (0001) planes. This conflicting face-selective behavior leads to inhomogeneous dopant distribution. Density functional theory (DFT) calculations reveal that such face-selective behaviors are interpreted in terms of the coordination structure of WO_4^{2-} ions on each ZnO crystal plane. WO_4^{2-} ions coordinated on $(10\bar{1}0)$ plane with unipodal or bipodal bonds serve as surfactant for attracting Zn ion species, whereas those coordinated on (0001) plane with tripodal bonds are easily incorporated into nanowire as dopant. Upon our findings, we successfully demonstrate the rational control over the morphology and the elemental doping of W-doped ZnO nanowire via modulating nucleation events and WO_4^{2-} ion adsorption with a recently developed concentration window principle. This study clearly highlights the essential importance to understand the coordination structure of metal ions for designing the hydrothermal metal oxide nanowire synthesis.



Reference: J. Liu *et al.* *Commun. Mater.* 1, 58 (2020) (Nature Publishing Group)