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Atomistic Studies of Semiconductor Nanowires

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Semiconductor nanowires (NWs) are quasi-one-dimensional nanostructures that have sparked a surge of interest as powerful and versatile building blocks for an extended range of emerging nanoscale technologies. These novel technologies exploit size-related effects, the flexibility in the fabrication and design offered by the use of NWs, and the concomitant progress in probing nanoscale properties. In this presentation, we will focus on NWs synthesized through VLS/VSS modes. More precisely, we will discuss the current understanding and technological implications of defect engineering and impurity incorporation into these NWs. The phenomenon of mass transport at the catalyst-nanowire interface will be elucidated. Particularly, catalyst atoms injection and trapping in NWs will be addressed. This phenomenon implies atoms detachment from the catalyst and their injection into the growing nanowire thus involving atomic scale processes that are crucial for the fundamental understanding of the catalytic assembly of nanowires. Herein, we present an atomistic level and quantitative study of this phenomenon of catalyst dissolution by three-dimensional atom-by-atom mapping of individual silicon nanowires using highly focused ultraviolet laser-assisted atom-probe tomography. This catalytic doping is described using a model of solute trapping at step edges and the key growth parameters are identified based on a kinetic model of step-flow growth of NWs. The control of this phenomenon provides myriad opportunities to create entirely new class of nanoscale devices by precisely tailoring shape and composition of metal-catalyzed nanowires.

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