

Tungsten-Based Intermetallic Compound as Catalyst for Structure-Specific Growth of Single-Walled Carbon Nanotubes

Professor

Yan Li

Visiting Professor, Department of Mechanical Engineering, The University of Tokyo Chang Jiang Professor, College of Chemistry and Molecular Engineering, Peking University

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Abstract

Single-walled carbon nanotubes (SWNTs) have shown great potentials in various applications attribute to their unique structuredependent properties. Therefore the controlled preparation of chemically and structurally pristine SWNTs is a crucial issue for their advanced applications (e.g. nanoelectronics) and has been a great challenge in more than two decades. The composition and morphology of the catalyst nanoparticles and the property of the catalyst supports were widely reported to affect the structure of SWNTs produced. In this talk, I will discuss the strategy in catalyst design for the structural controlled growth of SWNTs. Different from the conventional mono-metal catalysts, tungsten-cobalt intermetallic compound W₆Co₇, which belongs to monoclinic crystal system, presents lower structural symmetry and a very unique atomic arrangement. Therefore, W₆Co₇ exhibits specific geometry match towards the end structures of single-walled carbon nanotubes (SWNTs). This kind of one-by-one recognition between a crystal plane to a certain chirality of SWNTs enables this tungsten-based intermetallic compound an efficient template for structure-specified growth of SWNTs. This idea was revealed by both DFT simulation and the result of chemical vapor deposition growth of SWNTs. The manipulation of the structures of the W₆Co₇ catalysts was also performed to meet the requirements of the selective growth of SWNTs with different chiralities.



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