**Abstract**

Spectroscopy Insight in the Nickel Catalyst State in Carbon Nanotube Growth inside Metallic Single-Walled Carbon Nanotubes †

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The catalyst state in carbon nanotube growth is metal or metal carbide. It is important to investigate the chemical state of catalysts. The applications of carbon nanotubes (CNTs) require detailed investigations of the structures and properties of catalysts. A novel factor of this work is that the chemical and physical properties of nickel catalysts in the growth of single-walled carbon nanotubes (SWCNTs) inside metallic SWCNTs were investigated. The difference to other works is that metallicity-sorted metallic SWCNTs were used as templates. The growth of carbon nanotubes was monitored in the outer template metallic SWCNTs where metallocenes served as catalysts and sources of carbon. This system provided as best as possible control over the synthesis conditions, and the processes of metallocene catalyst decomposition and metal carbide/metal formation were traced by X-ray photoelectron spectroscopy (XPS). It was found that the positions of Ni 2p XPS were tracked after heating metallocene-filled metallic SWCNTs. All states of nickel were studied in detail with increasing annealing temperature. We found that chemical reactions of molecules, metal carbides, and metals occurred inside metallic SWCNTs upon heating. First, at low annealing temperatures, metastable nickel carbides were formed. Second, at higher annealing temperatures, nickel carbides were transited into metallic nickel. Third, at high annealing temperatures, nickel was removed from SWCNTs.

**Keywords:** carbon nanotube; metallocene; growth; spectroscopy

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**Supplementary Materials:** The presentation materials can be downloaded at: [https://www.mdpi.com/article/10.3390/proceedings2024105010/s1](https://www.mdpi.com/article/10.3390/proceedings2024105010/s1).

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