High-resolution TEM study on internal metal-carbon interface in carbon nanotubes

A Kiessling1,2, D Pohl1,2, C Taeschner3, MH Ruemmel9, L Schultz1,2 and B Rellinghaus1

1. IFW Dresden, Institute for Metallic Materials, Dresden, Germany.
2. TU Dresden, Institute for Solid State Physics, Dresden, Germany

a.kiessling@ifw-dresden.de
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Since their discovery in 1991 by Iijima [1], carbon nanotubes (CNT) have attracted the interest of the scientific community due to a variety of exceptional physical properties such as, e.g., their hardness or their good electrical and thermal conductivity. Envisioned technological applications based on the use of CNT embrace, for instance, logic and memory devices, sensors, actuators and field emission devices.

Understanding the growth mechanism of CNTs is considered to play an important role for application purposes. In particular in the case of tip-functionalization of CNTs where the relative orientation between the CNT axis and the crystal lattice of the catalyst particle is a key requirement, a detailed knowledge of the nature of the interface between the graphene layers of the CNT and the catalyst particle is mandatory.

Recently, Pohl et al. have reported that in case of CNT grown from FePt catalyst nanoparticles the (111) facets are energetically favoured for the release of carbon [2]. The study shows that this preference is due to a reduction of the desorption energy for carbon atoms on the aforementioned facets.

In order to improve understanding of the physics that govern the growth of CNTs, carbon nanotubes were prepared from Fe20Ni80, Ni, Fe, Pt and Co catalyst nanoparticles via plasma-enhanced chemical vapour deposition (PECVD). The as-grown CNTs are then investigated by aberration-corrected high-resolution transmission electron microscopy (HR-TEM) using a FEI TITAN³ 80-300 microscope that is operated at 80kV in order to minimize defects induced by knock-on damage.

In case of Ni, theoretical studies utilizing the Modified Embedded Atom Method (MEAM) studies indicate that the facet to be considered the energetically favoured one is the (111) [3]. This preference is, however, weaker than in case of FePt. Our structural investigations based on statistical HRTEM studies, on the other hand, do not indicate any preference of a particular facet that would favourably interface the outgrown CNTs. Neither in the Ni nor in the Ni-rich Fe20Ni80 catalyst particles any signs of a “perpendicular” growth of the individual graphitic walls of the CNT from a metal surface as, e.g., indicated by a significant bending of the walls toward the metal [2] are found. Rather are the CNT walls always found to lie parallel to the surfaces of the catalyst particles (cf. Figure 1) thereby indicating a largely different growth mode as compared to CNT growth from FePt catalysts. The HRTEM investigations also reveal a significant distortion of the otherwise fcc structure of the Ni and Ni80Fe20 catalyst particles (cf. Figure 2) that goes along with an enhancement of the average atomic volume. The latter could be indicative of an increased carbon solubility in the likewise distorted lattice. The stronger tendency of Ni to form carbides as compared to Pt lends support to this assumption.

Results and comparisons with the other above mentioned systems will be discussed.
References


**Figure 1.** TEM image of a typical $\text{Fe}_{20}\text{Ni}_{80}$-catalyzed CNT. The graphitic walls of the CNT smoothly adapt to the curved morphology of the catalyst particle without revealing any indications of a pronounced bending towards its surface.

**Figure 2.** Left: Close-up of Figure 1. Right: The Fast Fourier-Transformation (FFT) of the region marked red in the TEM image (on the left) reveals a significant distortion of the lattice. The labeling of the Bragg peaks is in accordance with an fcc crystal seen along a $[110]$ zone axis. The yellow dots indicate the positions of the Bragg peaks of the undistorted fcc crystal.