Direct imaging and analysis of the internal interfaces between carbon nanotubes and their catalyst particles

D. Pohl[1], F. Schäffel[1], C. Täschner[2], M. H. Rümmeli[2], C. Kisielowski[3], L. Schultz[1], and B. Rellinghaus[1]

1. IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, Dresden, D-01171, Germany
2. IFW Dresden, Institute for Solid State Research, P.O. Box 270116, Dresden, D-01171, Germany
3. National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

d.pohl@ifw-dresden.de
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For the application of carbon nanotubes (CNT) in electronic devices as well as in novel composite materials a detailed understanding of both their structure and growth mechanism at the atomistic level are required [1]. The functionalization of the ends of the CNT has become an important research field due to the potential to hereby modify their electronic and magnetic properties [2,3]. Functionalized CNT can thus be used to build up new functional micro-scaled structures with high performance.

Owing to its large magneto-crystalline anisotropy energy, L10 ordered tetragonal FePt is among the most intensively discussed materials when it comes to pushing the superparamagnetic limit towards minimum particle sizes [4]. As a consequence, this material is of particular interest for the realisation of a hard-magnetic termination of the CNT. In the present study, plasma-enhanced chemical vapour deposition (PE-CVD) is used to synthesize CNT from a Fe-Pt multilayer catalyst thin film stack [5] with the aim to implement hardmagnetic
FePt nanoparticles at the end of the CNT. Likewise prepared CNT are characterized by means of aberration-corrected HRTEM. In order to gain a deeper insight into the growth mechanism these structural investigations are focused on the atomically resolved characterisation of the inner FePt-CNT interface.

CNT are extremely susceptible to radiation damage which is why any HRTEM investigations are to be conducted at acceleration voltages as low as 80 kV. Furthermore, since the inter-atomic distances at the particle-CNT interface may vary over a wide range, high spatial frequencies are required to atomically image these interfacial layers. Figure 1 (a) shows exemplarily a HRTEM micrograph of such a FePt-CNT interface as obtained on themonochromated, aberration-corrected *TEAM 0.5* microscope at the NCEM in Berkeley, CA, USA. The interface between the CNT and the FePt catalyst particle can be clearly observed (see Fig. 1 (a) ,(b)). First results on the details of the atomic structure of the interface between the CNT and the catalyst particle will be shown.

A detailed analysis of the magnified section of the interface area displayed in Fig. 1 (b) reveals a systematic increase of the lattice spacing upon approaching the particle-CNT interface. As can be seen in Fig. 1 (c), the {111} lattice spacings measured in the interface area in Fig. 1b, is larger close to the interface than it is in the depth of the particle. A similar near-surface lattice expansion was already observed in gas-phase prepared FePt nanoparticles which was attributed to a of Pt segregation towards the surface [6,7]. How the presence of carbon atoms influences this near-surface lattice relaxation is, however, still unknown.

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It can be seen from Figure 2 that the graphitic layers of the CNT are strongly bent towards the {111} layers of the FePt catalyst particles. Such a bending strain inside the CNT will in turn inevitably cause a significant counter-strain in the interface-near lattice of the particles. The results of the structural characterization of these interfaces will be compared with the thermodynamically favoured nucleation sites of the graphitic layers of the CNT.

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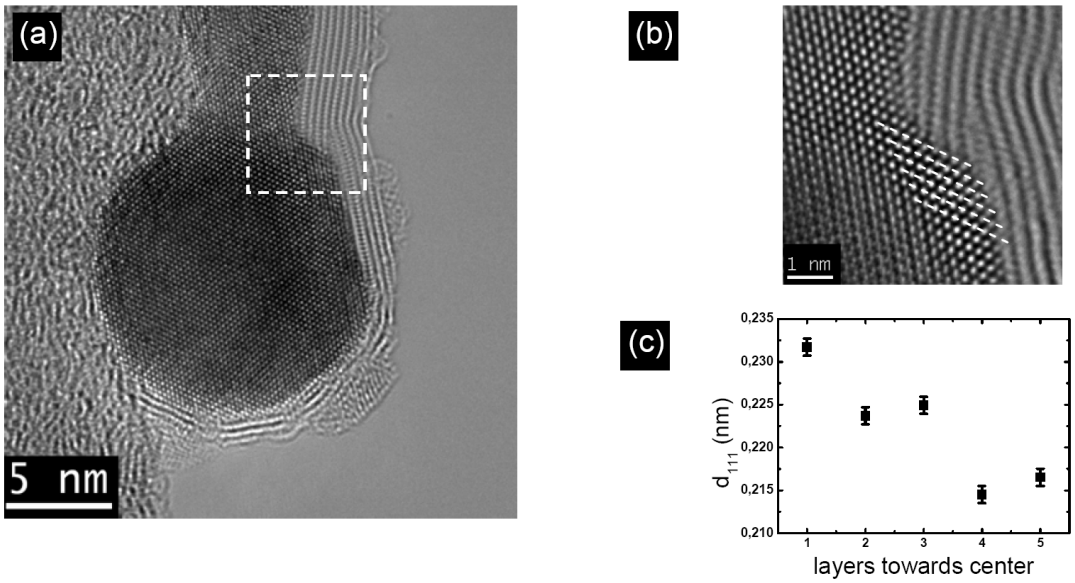

Figure 1. (a) Typical HRTEM micrograph of a multi-wall CNT with a FePt catalyst particle at the end inside the tube. (b) Magnification of the area marked in Fig. 1(a). Dashed lines indicate the measured layers.

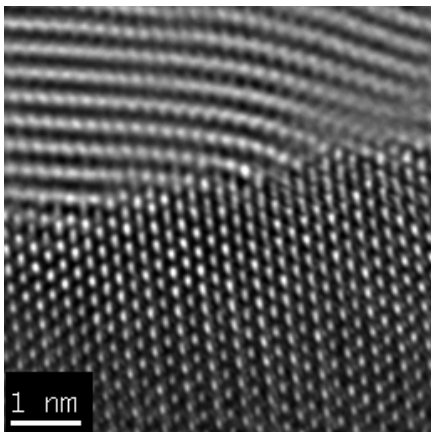

Figure 2. CNT-catalyst particle interface: The white arrow points to the near-interface area where a strong bending of the graphitic layers towards the FePt particle's {111} planes.