

# In-situ TEM investigation of interface dynamic behavior between carbon nanotube and metal-electrode

## Mingsheng Wang\*, Dmitri Golberg\*, Yoshio Bando

International Center for Materials Nanoarchitectonics, National Institute for Materials Science (NIMS), Tsukuba, 305-0044 Japan \*E-mails:WANG.Mingsheng@nims.go.jp, GOLBERG.Dmitri@nims.go.jp

### Abstract:

The end-to-end connection between an individual carbon nanotube (CNT) and a tungsten (W) nanoelectrode was made in situ in a transmission electron microscope. An analysis of the interface dynamics under a current flow and Joule heating was then performed. The interface transitions were directly observed and video-recorded under a nearly atomic resolution. The study uncovered direct evidence for the bulk diffusion of C through a W electrode. First, the W tip-end absorbs the source CNT atoms, which then penetrate deep into its body, form a carbide (Fig. 2a-d and Fig. 3a,b), and finally precipitate as freshly-formed graphitic tubular shells encapsulating the electrode (Fig.2e-g and Fig.3c-f). CNT wall-thickness shaping via stepwise soaking of the nanotube core shells into a W electrode is then demonstrated (Fig.4), and a selfselection mechanism based on a C concentration gradient is proposed. This work provides new and detailed understanding of the CNT catalytic growth, which is vital in developing novel and efficient nanotube syntheses. In addition, it shows the complexity of the atomic-scale diffusion/segregation processes at a CNT/metal electrode interface during a given nanoelectronic device exploitation; this so far has largely been hidden and/or underestimated. Lastly, hereby created one-dimensional nanotube-carbide-metal heterojunctions are mechanically robust and exhibit excellent transport properties, thus enhancing the prospects for future CNT-based electronic devices.





Figure. 1 Schematic diagram of the experimental setup inside TEM. The *in situ* soldering experiments were conducted with a Nanofactory TEM-STM sample holder operated performed in a JEM-3100FEF 300 kV field-emission high-resolution transmission electron microscope. Side contact with gold wire and end-to-end contact with W tip are established for the two CNT ends.

#### Results





**Figure 2.** Morphology and structure changes of a CNT/W junction under biasing and Joule heating. a-g. The series of low-magnification TEM images showing the structural transformation of the CNT-W (both with a diameter of ~25 nm) interface. **c-e**, The white arrows indicate the positions of the interface between the tungsten carbide and pure tungsten domains. **e-f**, Black arrowheads indicate the boundary of precipitated graphitic layers on the W tip surface: **g**, A carbon onion is finally found to be attached to the CNT surface; **h**, the corresponding *I-V* curves peculiar to the structures in **a-c**.



**Figure 3. Graphitic layers growth on the W electrode surface. a-f,** HRTEM images providing the structural details of the CNT-W interface in Fig. 2. The images in Fig. 3(a, b, e, f) correspond to the images in Fig. 2(c,d,e,f), respectively; **c-f,** the enlarged images of the indicated region in **b**, the numbers of graphitic layers counted are marked in **c-f.** All the scale bars are 5 nm.

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Figure 4. Selective stepwise innermost graphitic shells absorption into the W electrode. a-f, TEM images illustrating the stepwise extraction of the core shells from the source CNT. a, The original CNT has a diameter of 32 nm with a narrow hollow core. b, The innermost shells, ~3 nm in diameter, have already been absorbed. c, The second core shell package with an outer diameter of ~14 nm is partly and then totally d extracted. e, The third extracted set has an outer diameter of ~ 18 nm. f, The further ingestion of the outer shells leads to the CNT-W junction break. The arrows in c and e indicate the edges of the extracted shells.