TEM IMAGE SIMULATION: POWERFUL TOOL TO CHARACTERIZE CARBON NANOTUBES

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Introduction

Thanks to the improvement of the CCVD method, we are now able to produce sub-nanometer tube (subnanotube) such as 0.43 nm diameter tube as reported earlier [1], and thicker but still sub-nanometer tube (0.6 – 0.9 nm diameter) at a regular basis.

Analytical techniques for such sub-nanometer materials are limited to several techniques like transmission electron microscopy (TEM), Raman spectroscopy, and scanning probe microscopy. Among these methods, most of the studies related to nanotube and nanowires use TEM as an indispensable tool for analyzing the structure, diameter, and crystallinity of the sub-nanometer carbon materials.

But there is one thing we always have to be careful when using TEM on such small materials: the interference effect caused by the improper focus condition of the small materials, which result in ghost image (artifact) that appears in the TEM photographs. This problem applies to larger scale materials as well, but the danger of misinterpreting the image is small compared to the sub-nanometer materials that we are now treating.

In this study, we used the multi-slice TEM image simulation technique to investigate the effect of defocus amount to the TEM image of sub-nanometer carbon materials.

Experimental

TEM image simulation was performed with the multi-slice TEM simulation program integrated in Cerius[2]. The multi-slice method is the most commonly used image simulation method. Most of the simulating conditions (Acceleration voltage was 200 keV, Cs = 1mm) were set identical to our TEM (JEOL JEM-2010FEF) and is similar to most of the 200 keV TEM around.

We have performed the image simulation for the following models: 0.3nm carbon nanotube in the core of a MWCNT, same model without the 0.3nm tube, bundle of SWCNTs, and bundle of DWCNTs. Since there is an anisotropy in the bundle model, we have simulated for three different incident beam directions.

We have changed the defocus values and compared with the images of a typical carbon nanotubes. For the simulation involving 0.3nm carbon nanotube, we have simulated using 120 keV acceleration voltage.

Results and Discussion

The simulated results of a MWCNT with and without 0.3nm carbon nanotube are shown in Figure 1. With the 0.3nm tube core, we can find the contrast corresponding to the core in some defocus range, but not at the optimal defocus condition that is known to give highest resolution (-58nm). When we change the defocus value to –25nm, we can see the central layer that seems to correspond to the 0.3nm nanotube. Interestingly, in the image simulation without the core SWCNT at the same defocus range, we can see the parallel contrast at the hollow part that looks like a contrast of a tube although nothing is supposed to exist. This is the ghost image due to the fringe that appears at a certain defocus condition. It was only when we changed the simulation condition and raised the acceleration voltage to 1200keV, that we could clearly find the 0.3nm tube at the core at the optimal defocus condition (-28nm). This result shows that, we need an Ultra high-voltage TEM to obtain the information for such fine material like 0.3nm carbon nanotube.

SWCNT and DWCNT bundle simulation showed that at some defocus values, it is hard to tell whether the bundle consists of SWCNTs or DWCNTs (Figure 2).

Conclusions

By performing the image simulation for various models consisting of carbon nanotubes, we have shown that we have to be cautious about using the TEM, because the obtained result is still not that easy to understand. We suggest the use of image simulation, at least when what you are observing is simple enough, to help understand what we are looking.

References

[1] T. Hayashi, Y.A. Kim, T. Matoba, M. Esaka, K. Nishimura, T. Tsukada, M. Endo, M.S. Dresselhaus, *Nanoletters* **3**, 887 (2003)

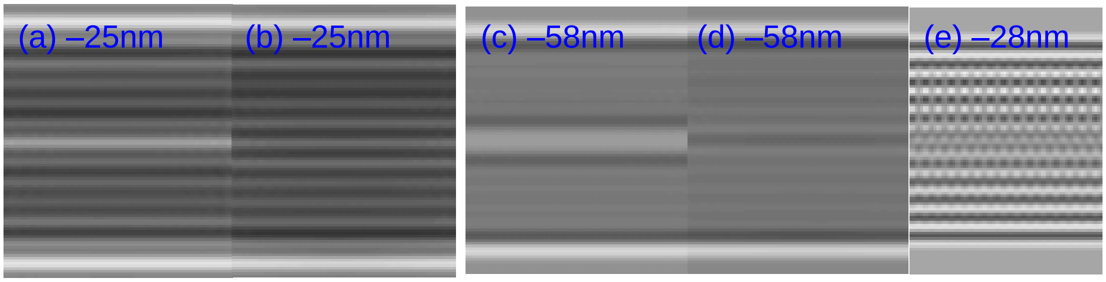

Figure 1 Simulated images of MWCNT without 0.3nm nanotube at the core (a, c) and with 0.3nm nanotube core (b,d). Simulated image under 1200keV condition is shown in (e)

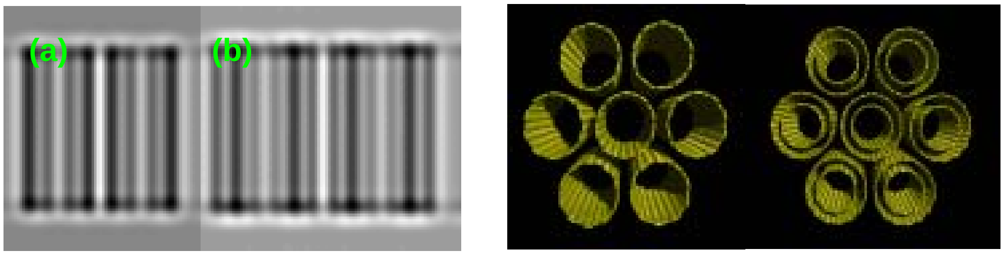

Figure 2 Simulated images of SWCNT bundle and DWCNT bundle. Can you tell which is which? (a) is the SWCNT bundle, and (b) is the DWCNT bundle.