doi:10.1017/S1431927611008440
Microsc. Microanal. 17 (Suppl 2), 2011

Electron Diffraction Study of Individual C_{60}@SWCNT Peapods

K. Ran,[1,2] Q. Chen,[2] X. Mi,[3] Y.F. Shi,[3] J.M. Zuo[1]

[1] Department of Materials Science and Engineering and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1304 W Green Street, Urbana, IL 61801
[2] Department of Electronics, Peking University, Beijing, P. R. China 100871
[3] Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, 110 8th Street, Troy, NY 12180

C_{60} molecules encapsulated inside single-walled carbon nanotubes (SWCNT)[1], the so-called peapod, has received significant research interests as a truly one-dimensional molecular structure and a model system for the study of a hybrid nanomaterial with unusual electronic and structural properties.

With the encapsulation of C_{60}s, a pressure of an order of Gpa is expected within the host SWCNT. This pressure is expected to compress the fullerenes and result in a smaller inter-fullerene spacing than in bulk crystals.[2] Published high resolution TEM images, as well as diffraction patterns recorded from peapod bundles, provided some experimental evidence for the compression. However, these results were averaged among different peapods and the results were also dependent on the tube tilt and subjected to the limit of the microscope's resolution. Ordered phases of C_{60}s inside SWCNT were predicted based on molecular dynamic simulation.[3] It was pointed out that the arrangement of C_{60}s is mainly dependent on diameter of the host SWCNT.

We have investigated the structure of C_{60}@SWCNT peapod by electron imaging and diffraction at 80 kV. Experiment was performed using the JEOL2200FS electron microscope at University of Illinois. The microscope has a Cs probe corrector and UHR pole piece for electron imaging [4]. 80 kV was selected to reduce radiation induced beam damage to the single-walled carbon nanotubes. Molecular motions of C_{60}s molecules were observed under prolonged electron beam exposure for peapods with C_{60} vacancies or defects [5]. Electron diffraction patterns were recorded using a 25 nm diameter parallel beam (Figure 1b) formed using the settings described in the ref. [4].

We recorded diffraction patterns from ~40 isolated peapods. Among these, 5 of diffraction patterns contain clear C_{60}s diffraction information (an example is shown in Figure 2). The diffraction information of the host SWCNT is also clear in the recorded patterns, which allows a structure analysis using the established nanotube structure analysis methods [6,7]. Using the diffraction pattern of SWCNT as a reference, we developed a method to measure the average separation between neighboring C_{60}s in the one dimensional molecular chain.

Furthermore, we have simulated the structure of peapods using molecular dynamics with classical potentials. Consistent with the experimental observation, simulation by molecular dynamics indicates, that C_{60}s' packing is very sensitive to the diameter of the host nanotube. Large diameter (>15 Å) leads to off-axis packing of C_{60}s, and further results in missing of C_{60}s' intensity in peapod diffraction pattern, as we observed in the other diffraction patterns. Both experimental and theoretical results will be discussed in this presentation.[8]

References

[1] B. W. Smith et al., *Nature* 396 (1998) 323.
[2] K. Hirahara et al., *Phy. Rev. B* 64 (2001) 115420.
[3] B. Verberck et al., *Phy. Rev. B* 74 (2006) 045421.
[4] J.G. Wen et al., *Microsc. Microanal.* 16 (2010) 183.
[5] K. Ran et al. Submitted to *ACS NANO*. (2011).
[6] J.M. Zuo et al., *Microsc. Res. Techniq.* 64 (2004) 347.
[7] J.M. Zuo et al., *Z. Kristallogr.* 222 (2007) 625.
[8] This work was supported by NSF of China (60728102 and 60925003) and DOE (DEFG02-01er45923). K. R. acknowledges fellowship support from CSC (China). Microscopy was carried out at the Frederick Seitz Materials Research Laboratory Central Facilities, University of Illinois.

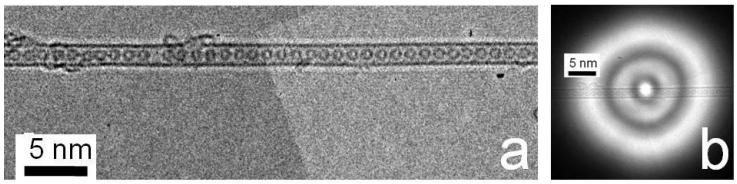

FIG.1 (a) TEM image of an isolated peapod. (b) Electron beam used for diffraction

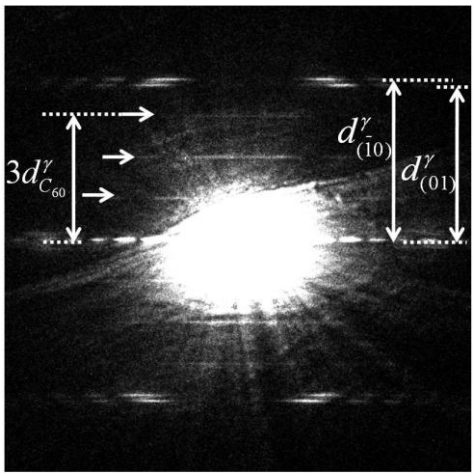

FIG. 2 Diffraction pattern from the peapod shown in FIG. 1.

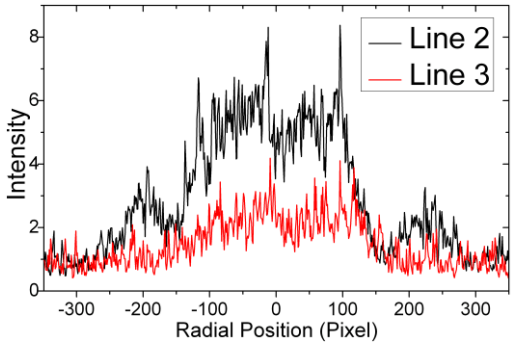

FIG. 3. C_{60}s' intensity distribution in the peapod diffraction pattern.

https://doi.org/10.1017/S1431927611008440 Published online by Cambridge University Press