

## Electron Diffraction Study of Individual C<sub>60</sub>@SWCNT Peapods

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C<sub>60</sub> 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<sub>60</sub>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<sub>60</sub>s inside SWCNT were predicted based on molecular dynamic simulation.[3] It was pointed out that the arrangement of C<sub>60</sub>s is mainly dependent on diameter of the host SWCNT.

We have investigated the structure of C<sub>60</sub>@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<sub>60</sub>s molecules were observed under prolonged electron beam exposure for peapods with C<sub>60</sub> 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<sub>60</sub>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<sub>60</sub>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<sub>60</sub>s' packing is very sensitive to the diameter of the host nanotube. Large diameter (>15 Å) leads to off-axis packing of C<sub>60</sub>s, and further results in missing of C<sub>60</sub>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

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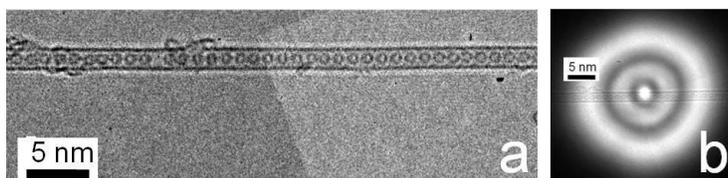


FIG.1 (a) TEM image of an isolated peapod. (b) Electron beam used for diffraction

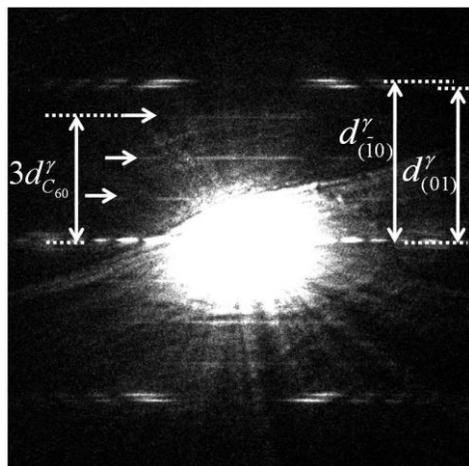


FIG. 2 Diffraction pattern from the peapod shown in FIG. 1.

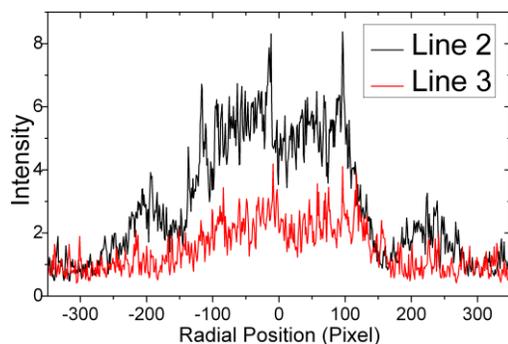


FIG. 3.  $C_{60}s'$  intensity distribution in the peapod diffraction pattern.