PRESSURE-INDUCED STRUCTURAL TRANSITIONS IN MULTIWALL CARBON NANOTUBES

Hiroyuki Shima *and Motohiro Sato*
Department of Applied Physics, Graduate School of Engineering,
Hokkaido University, Sapporo 060-8628 Japan
shima@eng.hokudai.ac.jpl

An important mechanical feature of carbon nanotubes is their high flexibility in the radial direction. It has been found that the magnitude of radial stiffness of an isolated carbon nanotube is considerably less than that of axial stiffness, which allows a reversible change in the cross-sectional shape on applying a hydrostatic pressure. Such a pressure-induced radial deformation yields significant changes in electronic [1] and optical [2] properties, indicating the relevance of radial deformations in carbon nanotube applications.

Thus far, many experimental and theoretical studies have been carried out on radial deformations of carbon nanotubes induced by hydrostatic pressures [3], most of which have focused on single-walled nanotubes (SWNTs) and their bundles. Successive investigations have revealed flattening and polygonalization in the cross section of SWNTs under pressures of the order a few GPa. As compared to the intensive studies carried on SWNTs, those on multiwalled nanotubes (MWNTs) are lagging behind. Intuitively, the core-shell structure of MWNTs is thought to enhance the radial stiffness of MWNTs. However, when the number of concentric walls is much greater than unity, outside walls have large diameters so that external pressure leads to a mechanical instability in the outer walls. The latter fact implies the possibility of a new cross-sectional shape transition of MWNTs induced by hydrostatic pressure.

In this presentation, we demonstrate theoretically a novel radial deformation, called the radial corrugation, of MWNTs under hydrostatic pressure [4]. Theoretical analyses based on the continuum elastic theory have revealed that MWNTs consisting of a large number of concentric walls undergo elastic deformations at critical pressure $p_{\mathrm{C}} \sim$ 1GPa, above which the cross-sectional circular shape becomes radially corrugated. We found various corrugation modes can be obtained by tuning the innermost tube diameter D and the number of constituent walls N, which is a direct consequence of the core-shell structure of MWNTs. A phase diagram has been established to obtain the requisite values of N and D for observing a desired corrugation mode. It is remarkable that in all corrugation modes, the cylindrical symmetry of the innermost tube is maintained even under high external pressures. This persistence of the cylindrical symmetry of the innermost tube of MWNTs is completely in contrast to the pressure-induced collapse of SWNTs. We hope that the present results provide useful information for developing nanofluidic or nanoelectrochemical devices whose performance depends on the geometry of the inner hollow cavity of nanotubes.

References:

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