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Pressure- and temperature-induced structural changes of polyiodide ions encapsulated in single-walled carbon nanotubes

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1 Introduction

Owing to the unique inner surface potential of single-walled carbon nanotube (SWCNT), several kinds of molecules can be encapsulated in SWCNT hollow cores. Since the discovery of C_{60} peapods (C_{60} molecules encapsulated in SWCNTs) in 1998, several kinds of molecules (e.g. coronene, β-carotene, 9,10-dichloroanthracene, water, iodine) have been encapsulated so far. Some of the eager studies on physical and chemical properties of encapsulated molecules reported that some of the encapsulated molecules showed properties different from their bulk forms. Due to such findings, it has been concluded that the tube interior provides a unique field to the encapsulated molecules to alter their properties.

We have developed very simple electrochemical iodine doping method to encapsulate iodine molecules into single-walled carbon nanotubes (SWCNTs). It was found that the electric conductivity of SWCNTs is drastically improved by iodine encapsulation because many hole careers are introduced. It was also found that the SWCNTs encapsulating iodine molecules (I@SWCNTs) are well dispersed in water at low temperature.[1] However, structural properties of the encapsulated iodine molecules have not been clarified yet. Here we report on pressure- and temperature-induced structural changes of polyiodide ions encapsulated in SWCNTs.

2 Experiment

SWCNTs (Meijo Nano-Carbon, EC2.0 type) having mean tube diameter of ca. 2.5 nm were used. Iodine encapsulation treatments were done in an electrochemical cell consisting of SWCNT electrodes and NaI aq. electrolyte. High pressure experiments were done with diamond anvil cell. Synchrotron XRD measurements were performed at a beam line BL-18C of KEK. High energy X-ray of 20 keV was used as an incident beam and an imaging plate was used as a detector. Low temperature Raman measurements were also performed using a JASCO NRS-3300 spectrometer and a Linkam 10036L temperature control stage.

3 Results and Discussion

We observed three Raman bands in low wavenumber region. Here, we assigned the peaks observed at around 110, 165, and 175 cm^{-1} as the frequency modes of polyiodide ions I_3^-, I_5^- and I_7^-, respectively. As shown in Fig. 1, the peak intensity of I_7^- ions increased with decreasing temperature. It indicates that structural transformations from short molecules to long molecules are promoted at low temperature. On the other hand, it was found that the peak intensity of I_3^- ions increases with pressure. In order to explain these structural changes of poly-iodide ions, we should analyze the XRD patterns observed under high pressure.

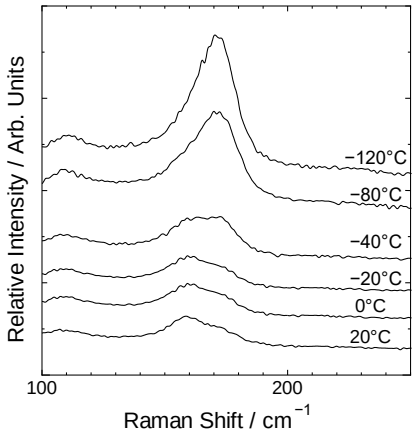

Fig. 1: Change in Raman spectrum of I@SWCNT with decreasing temperature.

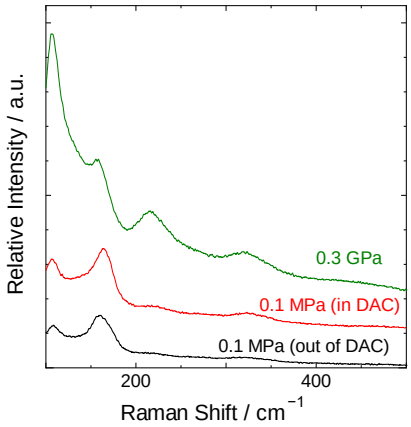

Fig. 2: Change in Raman spectrum of I@SWCNT with increasing pressure.

References

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[2] Y. Taniguchi et al., J. Nanosci. Nanotechnol., in press.

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