# [Grant-in-Aid for Scientific Research(S)] Science and Engineering (Interdisciplinary science and engineering)



Title of Project : Physical Properties and Applications of Fully Structure Controlled Carbon Nanotubes

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Research Area : Materials science, Nano science

Keyword : Nanotubes and graphene, Separation, Single crystal

[Purpose and Background of the Research] Single-wall carbon nanotube (SWCNT) was discovered in Japan in 1993. It is one-atom-thick layered cylindrical carbon material having a few nanometers in diameter. Because of its superior physical and electrical properties, various applications have been proposed to date. However, even accurate C-C bond lengths have not been provided yet though twenty years have passed from its discovery. This is because we could not get a single crystal of SWCNT. Because SWCNT is always produced as a mixture of dozens of structural isomers, a growth of mono structured SWCNT single crystal could not be achieved.

In this study, we will prepare high-purity mono structured SWCNTs in large quantity by sorting the mixture solution using a new gel column chromatography that we developed. Then we grow a single crystal of SWCNT. Once we could get a single crystal, we can determine the precise C-C bond lengths by X-ray diffraction analysis. We will realize these conventional but fundamental studies for SWCNTs using the single crystals.

# [Research Methods]

Our separation method of SWCNT is quite unique in which we use an agar gel, a traditional food in Japan. This kind of gel has a selective affinity to SWCNT of specific structure, which we can use for separation although the detailed mechanism is still unknown. In this study, we will design and build a new separation apparatus for



200ml Column

Figure 1 Gel column under the separation (left). Aqueous solution and structure model of separated mono structured (6,5) SWCNT (right). Nano Lett. (2013)

the large scale separation of the mono structured SWCNT, and try to grow the single crystals.

Figure 1 shows a gel column under the separation of so-called (6,5) SWCNTs. Usually, SWCNT is thought to be a black material, but the mono structured SWCNT shows a clear color like the other nano materials. We have already succeeded to get thirteen kinds of mono structured SWCNTs. In this study, we will try to improve the number and the purity.

### [Expected Research Achievements and Scientific Significance]

Energetics calculation predicted a breakdown of periodicity the long range because of a spontaneous torsion for the chiral SWCNT. We can confirm this issue as well as C-C bond lengths measurements by the precise structural analysis using the single crystal of SWCNT. Furthermore, mono structured SWCNT single crystal can be regarded as a new solid phase of pure carbon. We can prepare many kinds of new solid phases which have different energy structures. In this system, new superconducting phases could be expected just like alkali metal doped graphite and fullerene crystals.

# [Publications Relevant to the Project]

"Large-scale single-chirality separation of single-wall carbon nanotubes by simple gel chromatography", H. Liu *et al.*, Nat. Commun. **2** (2011) 309.

"High-Efficiency Single-Chirality Separation of Carbon Nanotubes Using Temperature-Controlled Gel Chromatography", H. Liu *et al.*, Nano Lett. **13** (2013) 1996.

**[Term of Project]** FY2013-2017

**(Budget Allocation)** 167,500 Thousand Yen

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