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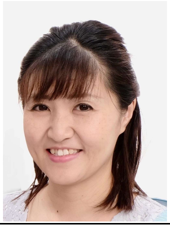

Maximizing the internal tube space of single-walled carbon nanotubes by selective removal of end caps

The internal tube space of single-wall carbon nanotube (SWCNT) provides a very strong attractive interaction potential for gaseous molecules even for supercritical gases, which induces the highly dense adsorbed layer formation inside the SWCNTs spaces[1]. However, the caps on both ends of prepared SWCNT are closed and it need to be removed without damaging the tube wall for utilizing the internal tube space. In this study, we studied the optimal conditions for cap-removal to maximize the internal tube space of SWCNT by air oxidation and a new method to determine the opening ratio using reliable specific surface area (SSA)[2] evaluated by the subtracting pore effect (SPE) method[3].

SWCNTs were thermally oxidized in air at different temperatures ranging from 623 to 823 K. The porosity of the oxidized SWCNTs was determined with nitrogen adsorption at 77 K. The SSA and microporosity were evaluated by the SPE method using a high-resolution α_s-plot[3]. The crystallinity change of SWCNTs due to oxidation was evaluated from Raman spectroscopy.

The air oxidation at 773 K of SWCNT bundles obtained a maximum surface area of 1840 m^2 g^{-1} without damaging the graphene walls of SWCNTs. The cap opening percentage of SWCNT is 98 % by comparing geometrical and observed SSA values. The selective removal of SWCNT end-caps can provide a new pathway for the highly selective modification of SWCNT bundles[4] utilizing the internal tube space.

1) (a) K. Kaneko *et al.*, *J. Chem. Phys.*, **87**, 776-777 (1987). (b) K. Urita e*t al., J. Am. Chem. Soc.*, **133**, 10344-10347 (2011). (c) T. Fujimori *et al.*, *Nat. Commun.* **4**, 2162-2169 (2013). 2) A. Furuse *et al.*, *Adsorption*, **29**, 1-7 (2023). 3) S. Wang *et al.*, *Carbon* **175**, 77–86 (2021). 4) Y. Kawamata *et al.*, *J. Phys. Chem. C*, **128**, 12632-12641, (2024).