Dynamic Adsorption Behavior of Surfactants on Single-Wall Carbon Nanotubes in Aqueous Media by Experimentation and Molecular Dynamics Simulation

Daiki Minami*,†, Satoshi Horikoshi**, Kenichi Sakai*,**, Hideki Sakai*,** and Masahiko Abe*,**

*Faculty of Science and Technology, Tokyo University of Science (2641 Yamazaki, Noda, Chiba 278-8510, Japan)
**Research Institute for Science and Technology, Tokyo University of Science (2641 Yamazaki, Noda, Chiba 278-8510, Japan)
†Corresponding Author, E-mail: j7208709@ed.noda.tus.ac.jp

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Abstract

The adsorption behavior of surfactant molecules on the hydrophobic surface of single-wall carbon nanotubes (SWNTs) was examined experimentally by measurement of turbidity degree and average size of dispersed SWNTs aggregate, and the molecular dynamics (MD) techniques. Sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB) were used as model surfactants in aqueous media. The dispersion of SWNTs was investigated by MD simulation using the adsorption model of the surfactant on the SWNT surface. As a result, we found the clear difference of the adsorption behavior according to the kind of surfactants. The hydrophilic head group of SDS molecule adsorbed on the hydrophobic surface at the initial step of adsorption and the hydrophobic moiety of SDS repeated the adsorption and desorption on the surface. In contrast, the CTAB molecule formed the stable adsorption state on the hydrophobic surface. This adsorption behavior of surfactant molecule on the SWNTs surface affects the dispersion of SWNTs in aqueous media.

Key-words: Single-wall carbon nanotube, Surfactant, Sodium dodecyl sulfate, Cetyltrimethylammonium bromide, Molecular dynamics simulation

1. Introduction

Carbon nanotubes (CNTs) possess important properties derived from a combination of unique dimensional, structural and topological features. CNTs have become a focus in chemistry, physics and material science due to superior mechanical, electrical and thermal properties1). However, the aggregation of CNTs is easily progressed by the van der Waals force on CNT surface2,3). Therefore, the function for CNTs was decreased by aggregation of tubes. A variety of dispersion methods have been researched. Especially, surfactant-assisted dispersion of CNTs was used with an ultrasonication4). The dispersion of CNTs with some kinds of surfactants has been reported5-7). The clarification of the adsorptive behavior of the surfactant on the CNT surface is necessary for the selection of optimum surfactant.

In this short article, single-wall carbon nanotubes (SWNTs) were used as a model dispersion of CNTs. SWNTs were dispersed by the ultrasonic irradiation in aqueous surfactant solution. The adsorptive behavior to the surface of SWNT of the surface-active agent at this time was examined from the experimental data and the molecular kinetic computer simulation. The difference between dynamic adsorption behaviors of different surfactant molecules on the SWNTs surface was discussed from the results of experimental and computational investigation.

2. Materials and Methods

Ground single-wall carbon nanotubes (SWNTs) were provided by Nikkiso Co., Ltd. Sodium dodecyl sulfate (SDS; cmc 8 mM8)) and cetyltrimethylammonium bromide (CTAB; cmc 0.92 mM 9)) were used as a model surfactant. The surfactant solution used the concentration around the critical micelle concentration (4.0, 8.0 and 16 mM for SDS and 0.1, 0.5 and 1.0 mM for CTAB). In advance, the entwined SWNTs fiber was roughly untied with an Alex 1505 sonication bath (40-kHz frequency; 150 Watt power) by 60-min irradiation. Aqueous surfactant solution (50 mL) containing SWNT powders (0.2 mg) were dispersed with a US-300T homogenizer Nihonseiki Kaisha Ltd. Japan (20-kHz; 300 W).

The turbidity degree of SWNTs in the aqueous surfactant solution was measured by the temporal changed of UV-absorbance intensity at 262-nm10) with an Agilent Technologies 8453 UV-vis spectrometer. The interval for measurement of UV-absorbance after the ultrasonic irradiation was strictly fixed. The size distribution of SWNTs was analyzed using dynamic light scattering (DLS) technique with a Nicomp 380 ZLS (Particle Sizing Systems Co.). The solutions were allowed to stand for 30 min before DLS measurement and the DLS measurement was continued for