Information from XAS Spectra on the Interaction between Titania and CNT for Photocatalytic Purpose

Yu-Ling Wei (魏玉麟) and Jing-Yi Yang (楊靜怡)

Department of Environmental Science and Engineering, Tunghai University, Taichung, Taiwan

TiO_2-based nanocatalysts from sol-gel process usually have the agglomeration problem, leading to a decrease in reactive surface area. Among many substrates to disperse TiO_2, CNT has attracted much attention because of its chemically inertness, high mechanical strength, mesoporous hollow core allowing enough free space for diffusion of reactants and products, reasonable surface area, excellent thermal and electrical conductivities to readily convey electrons away from holes, thereby delaying the recombination of electron-hole pair. Moreover, its price has recently been enormously decreased to a level where large-scale commercial application can be implemented.

Figure 1 shows the SEM morphologies from as-prepared titania, titania grown and coated on CNT, and mixture of titania with CNT. The titania particles in the as-prepared titania and mixture of titania with CNT form agglomerates and have similar size, while for the titania grown and coated on CNT, titania particles appear to be well dispersed with much smaller size.

According to the TEM images, the preparation of modified CNT was achieved with nitric acid under microwave-assisted heating. The CNT sample was open-end, and the carboxylic group has been formed on its surface, and the impurities were oxidized away during the surface modification process. Discontinuous phase of Titania nanoparticles are observed to be dispersively coated on CNT. Although this study used Raman spectroscopy to study the samples of as-prepared titania, acid-modified CNT, titania grown and coated on CNT, and mixture of titania with CNT. No significant information can be extracted from the spectra in aspects of Raman shift. Further, the I_G/I_D ratios from all the above samples are non-distinguishable. Raman technique does not give the present study any evidence of chemical bonding between titania and modified CNT.

A comparison of the XANES spectra and their corresponding derivative spectra of as-prepared titania, titania grown and coated on CNT, and mixture of titania with CNT with two titania references, anatase and rutile phases reveals that the titania in as-prepared titania, titania grown and coated on CNT, and mixture of titania with CNT samples is present in anatase form.

The first-shell structural results of Ti were extracted from the fitting of the Fourier transformed EXAFS of all titania-containing samples. The as-prepared titania and mixture of titania with CNT samples are almost non-distinguishable in Ti $N_{1st\text{-}shell}$ value ($N_{1st\text{-}shell}$ = 4.70–4.90) and Debye-Waller factor (about 0.0057 $Å^2$); however, titania grown and coated on CNT has greater $N_{1st\text{-}shell}$, about 5.70 with an increased Debye-Waller factor (about 0.009 $Å^2$). The variations in molecular structural parameters are suggested to be due to the existence of chemical bonding between titania and modified CNT through the carboxylic group. Thus the removal of electrons from holes upon light irradiation explains the better photocatalytic activity of the titania on CNT in dye decomposition.

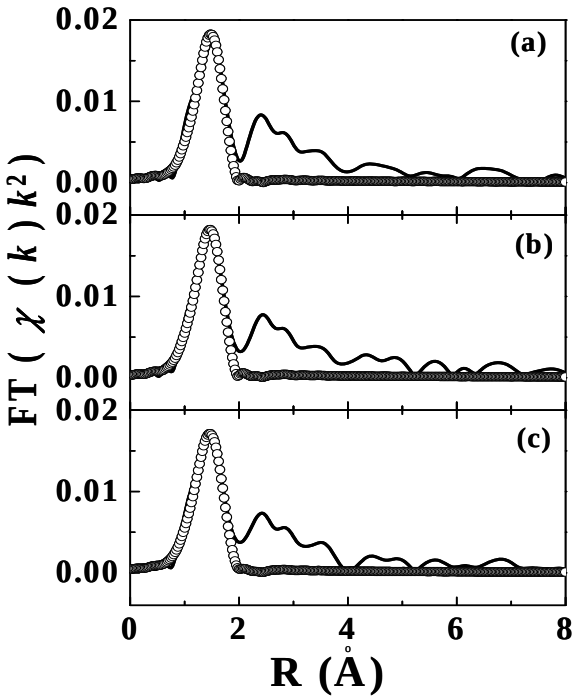

Fig. 1: Single-shell fitting of EXAFS spectra from (a) as-prepared titania, (b) mixture of titania and CNT, and (c) titania on CNT, and their simulated EXAFS spectra.

References

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