# Isotropic pitch-based carbon fiber analyzed by spectroscopies and computations

Yasuhiro Yamada[1], Takahiro Senda[1], Masakazu Morimoto[2], Toshiaki Sogabe[2], Noriko Nono[2], Shingo Kubo[3], Satoshi Sato[1]

[1]Graduate School of Engineering, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan

[2]Osaka Gas Chemicals Co., Ltd., 5-11-61 Torishima, Konohana, Osaka, 554-0051, Japan

[3]Research Support Center, Kagoshima University, 1-21-40 Korimoto, Kagoshima 890-0065, Japan

Isotropic pitch-based carbon fiber has been utilized for various applications such as thermal insulation materials for high-temperature furnace and additives for slide member, but the structure of the carbon fiber is still under debate. One of the reasons is that the precursor pitch contains various aromatic compounds in addition to oxidation and carbonization reactions, generating various defects in the carbon fiber. Another reason is that conventional analytical techniques using only the reported assignments of spectroscopies such as Raman, infrared-ray (IR), and X-ray photoelectron spectroscopy (XPS) are insufficient to understand the complicated structure of the carbon fiber. In this work, oxidation processes of model compounds of pitch such as pyrene ($sp^2CH$ with zigzag-like edges), triphenylene ($sp^2CH$ with armchair edges), fluorene (pentagon with $sp^3CH_2$), and 9-methylanthracene (hexagon with $sp^3CH_3$) were analyzed using mass spectrometry, elemental analysis, infrared (IR), Raman, and X-ray photoelectron spectroscopy (XPS) in addition to calculation such as molecular dynamic simulation with a reactive force field (ReaxFF) and simulation of IR, Raman, and XPS spectra (Gaussian09). Carbonization mechanism of isotropic pitch was further analyzed using similar techniques. Combination of calculations and experiments revealed that oxidation proceeded in the order of zigzag-like edges > $sp^3CH_3$ > $sp^2CH_2$ > armchair edges, and the quinone formed by oxidation worked as a precursor for a crosslinking reaction. Experimental and simulated results suggested that various defects with pentagon, heptagon, and oxygen-containing groups are present at 1073 K. Further heat treatment above 1073 K reduced oxygen-containing functional groups and remained defects such as non-hexagonal rings and edges such as non-TRIO and -QUATRO.