Quantitative analysis of zigzag and armchair edges on carbon materials with/without pentagons using infrared spectroscopy

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Infrared spectroscopy (IR) has been known to be capable of identifying such edge structures, quantitative analysis using IR spectra has been conducted using only out-of-plane sp^2C-H bending vibration and the estimation of the percentage of edges is still challenging. In this work, a novel two-dimensional method to quantify edge structures of carbon materials with/without pentagons was developed by analyzing both out-of-plane sp^2C-H bending and in-plane sp^2C-H stretching vibration. Twenty-two aromatic compounds with various edges were used as reference compounds to obtain peak positions of edges and intensities of the peaks for qualitative analyses of diffuse reflectance infrared Fourier transform spectra and to obtain calibration factors for quantitative analyses. For two-dimensional analyses using combination of two types of vibrations, a geometric mean was obtained by multiplying calibrated areal percentage of bending vibration and stretching vibration of edges.

Peak positions for each edge were obtained from experimental peak positions in this work. Contrary to the reported work, which exhibited only the calculated peak positions, this work clearly showed the experimental peak positions. Peaks originated from the out-of-plane sp^2C-H bending vibration have been utilized to classify the presence of each edge structure clearly, but correlation coefficients for out-of-plane sp^2C-H bending vibration were lower than those for in-plane sp^2C-H stretching vibration because of the coupled vibration for out-of-plane sp^2C-H bending vibration. Thus, these two vibrations were combined to improve the reliability of quantitative analysis.