Raman parameters of carbonaceous material estimated from fully-automatic spectral fitting method and their relation to vitrinite reflectance

*Shunya Kaneki[1], Yoshihiro Nakamura[2], Yui Kouketsu[3], Hideki Mukoyoshi[4]

1. Disaster Prevention Research Institute, Kyoto University, 2. Geological Survey of Japan, National Institute of Advancecd Industrial Science and Technology, 3. Graduate School of Environmental Studies, Nagoya University, 4. Graduate School of Science and Engineering, Shimane University

Carbonaceous material (CM) is widely distributed in sedimentary and metamorphic rocks, and its thermal maturity and crystallinity have been used as an indicator of burial and metamorphic temperature history. The relationship between maturity and temperature history of CM has been documented by various analytical techniques, including X-ray diffraction measurements, vitrinite reflectance measurements, transmission electron microscopy, infrared spectroscopy, and Raman spectroscopy. Among these, Raman spectroscopy is increasingly being used because of its rapidness and usefulness, as well as it is normally non-destructive technique (Henry et al., 2019).

A typical Raman spectrum of CM exhibits two distinct peaks of D (around 1350 cm^{-1}) and G bands (around 1580 cm^{-1}) (Tuinstra & Koenig, 1970). Various spectral parameters, which is associated with the thermal maturity of CM, are reported; e.g., intensity ratio and full-width at half maximum (FWHM) of D and G bands. Importantly, there are mainly two types in these spectral parameters: (1) parameters calculated from raw data, or (2) parameters calculated by performing spectral fitting. One of the representative parameters of the latter was proposed by Beyssac et al. (2002). Because it is argued that their R2 ratio (area of G band / area of D1+D2+G bands) is closely related to the CM maturity, numerous studies adopted the R2 ratio as a representative parameter of Raman spectra of CM (e.g., Kouketsu et al., 2014). On the other hand, Henry et al. (2018) suggested that spectral fitting should not be performed because it leads to unnecessary errors, and recommended to focus on the parameters that can be calculated from the raw spectrum without spectral fitting.

In the light of these backgrounds, the final goal of this study is to investigate whether spectral fitting of Raman spectra of CM is useful to evaluate its thermal maturity. As a first step toward this purpose, we developed a Python script that automatically perform spectral fitting of Raman spectra of CM. Analytical procedures of the script mainly consist of 5 parts: (i) smoothing by Savitzky-Golay filtering method, (ii) background correction with 1^{st} or 3^{rd} order polynomial function, (iii) normalization, (iv) setting of initial spectral parameters, and (v) non-linear spectral fitting with pseudo-Voigt function. We analyze the published data of Raman spectra of CM by Kouketsu et al. (2014), Mukoyoshi et al. (2018), and Nakamura et al. (2019), and compared the calculated parameters with the reported values of vitrinite reflectance. We will show preliminary results of our attempts in this presentation.

Keywords: Carbonaceous material, Raman spectroscopy, Spectral fitting, Vitrinite reflectance

