

Raman spectra of carbonaceous material in low-grade thermally-metamorphosed accretionary complex

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Sedimentary rocks contain a trace amount of initially poorly ordered carbonaceous material (CM), which transforms into well-ordered graphite with increasing metamorphic grade. Previous study has demonstrated that peak metamorphic temperature (T) can be estimated by an area ratio R2 (=D1/[G+D1+D2]) of peaks recognized in Raman spectra of CM. This geothermometer can be used at temperature range of 330-650°C (e.g., Bayssac et al., 2002; Aoya et al., 2010). Herein, we present Raman spectra from a suite of samples with different metamorphic temperatures which are estimated by a vitrinite reflectance method: Miocene Hota complex (50°C) (Yamamoto et al., 2005), Cretaceous Shimanto complex (150°C and 230°C) (Mukoyoshi et al., 2006) and Jurassic Ashio complex (300°C). First-order Raman spectrum of CM often decomposed into four peaks of a Raman shift (G peak at about 1580cm⁻¹, D1 peak at about 1350cm⁻¹, D2 peak at about 1620cm⁻¹, D3 peak at about 1500cm⁻¹). In our amorphous CM (coal) samples we recognized other three peaks on the D1 peak around 1150 cm⁻¹, 1220 cm⁻¹ and 1450 cm⁻¹. These peaks has been also reported in (e.g., Bar-Ziv et al., 2000; Zaida et al., 2007; Potgieter-Vermaak et al., 2011).

The first-order Raman spectrums of our coal samples, in particular low-temperature samples, are hard to fit with decomposed four peaks using the LabSpec program due to the influence of faint shoulders on D1. Therefore, there is no clear correlation between T and average R2 ratio in each sample. However, the Raman spectrums can be fit with the above seven peaks. The correlation between R2 and T can be described by the following exponential equation:

$$T (^{\circ}\text{C}) = 8.6 * \exp(7.0 * R2) \quad (R^2 = 0.98)$$

In addition, when we use an area ratio of D1/[decomposed seven peaks] which is referred to as R6 in this study, the correlation between R6 and T is given by

$$T (^{\circ}\text{C}) = 10.9 * \exp(11.9 * R6) \quad (R^2 = 0.99)$$

These correlations can be used for a potential geothermometer for low-grade metamorphosed sediments, in the temperature range of 50-300°C.

Keywords: raman spectroscopy, vitrinite reflectance, carbonaceous material, accretionary complex, geothermometry