Application Note

040-AN-004

Qualitative analysis of colorant by Raman Spectroscopy

<Introduction>

In order to progress Archeology, to study art history and to repair the works of art, it is generally very important to know and analyze what kind materials our ancestors used historically as colorant. Raman spectroscopy is a very useful technique especially for non-destructive analytical tool for qualitative analysis of archaeological ruins and works of art, because the measurement range is much wider than IR spectroscopy, enabling the measurement of not only organic colorant but also inorganic colorant that has absorption peaks in low wave number range below 400 cm^{-1}. It is considered to be difficult in general to obtain good Raman spectrum of the material which has fluorescent characteristic in UV region such as colorant, but it is possible to avoid this fluorescence emission effect without changing the excitation wavelength but keeping away from the absorption band because such materials have strong and sharp absorption peaks in visible region.
In this experiment, 12 different color water paint colorants were used as samples, which were excited by the lasers with 3 different wavelengths for comparative study.

<Experimental>

Instrument: JASCO NRS-3100 Laser Raman spectrometer
Samples: 12 different color water paint colorants
Objective lens: ×20
Excitation wavelength: 532 nm, 63 3nm, 785 nm

<Result and discussion>

Fig.1 shows the spectral data obtained in this experiment. As the result, Raman spectra of White, Yellow, Black colorants samples show the similar level S/N even excited by any of 3 different excitation wavelength. Spectra of Red, Lemon, Indigo blue, Scarlet, Brown and Ocher colorant samples show better S/N when excited by longer wavelength such as 785 nm, On the other hands, the better spectrum of Blue colorant sample was obtained when excited by the shorter wavelength such as 532 nm and also good spectra were obtained for Green, Yellow colorant samples excited by 633 nm. Table 1 shows colorant components of each samples as the result of this analysis. Generally, the color is recognized as the complementary color of absorbed light (Fig.2). As an example, Red colorant sample is considered to irradiate strong fluorescence when excited by 532 nm because it absorbs selectively the light between green and blue region. However, the Green colorant sample which is expected to absorb Red light has actually shown the best S/N condition when excited by 633 nm in Red region.

The cause of this phenomenon can be considered that Raman peak of Phthalocyanine compound(Fig.3) as the component of Green colorant sample is enhanced selectively by Red laser due to Resonance Raman effect. In addition the shapes of spectra of Green, Blue and Indigo Blue samples are different depending on excitation wavelength, which can be considered that the group vibration of Chromophore derived from absorption is enhanced selectively due to Resonance Raman effect. As well as Phthalocyanine, Chlorophyll and Hemoglobin which have similar chemical structure to Phthalocyanine are known as typical compounds that have Resonance Raman effect characteristics depending on excitation wavelength. Any spectra of Organic colorant which obtained in this experience could not be found in the liberally after searching. This is because the ratio of peak intensity is considered to be different depending on the excitation wavelength, which makes the spectra different from library data obtained by FT-Raman (1064 excitation) and Colorant components contain various crystal polymorph. Physical characteristics such as hue and anti-corrosion are different depending on the type of crystal Polymorph.
As shown in the above, Raman spectroscopy is one of the very useful analysis tool not only for colorant analysis, but also for evaluation of crystal polymorph and patent application for the cutting edge materials such as the luminescence material of Organic EL, absorbing colorant of Blue-Ray disk, and functional colorant as photovoltaic materials of Dye Sensitized Solar Cell.

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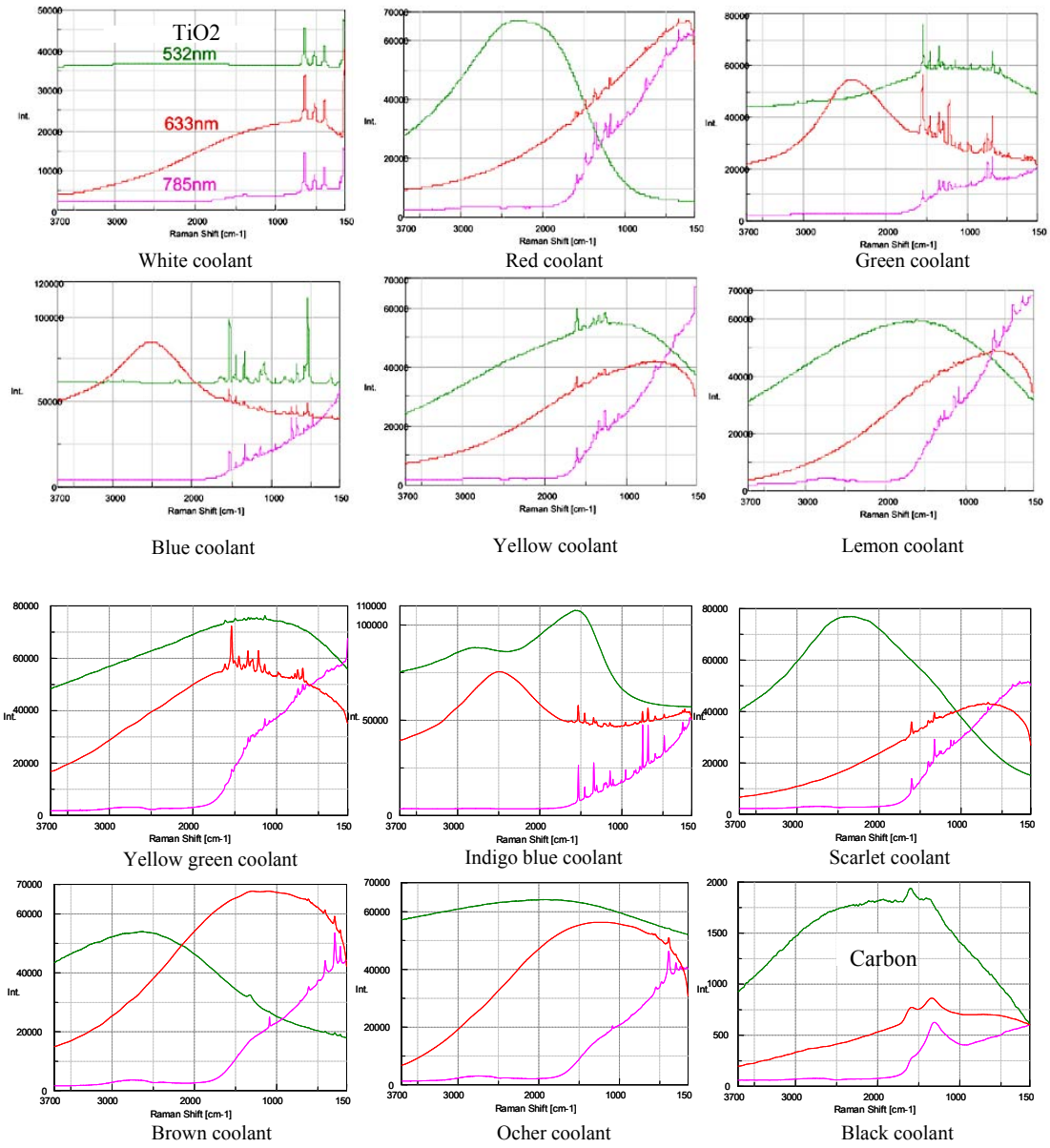

Fig1. Spectra data of colorant samples

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Colorant sample	White	Red	Green	Blue	Yellow	Lemon
Component	Titanium Oxide	Heterocyclic organic	Phthalocyanine	Phthalocyanine	Heterocyclic organic	Heterocyclic organic
Colorant sample	Yellow Green	Indigo Blue	Scarlet	Brown	Ocher	Black
Component	Phthalocyanine	Phthalocyanine	Heterocyclic organic	Inorganic	Inorganic	Carbon

Table 1.Analysis result of Colorant component

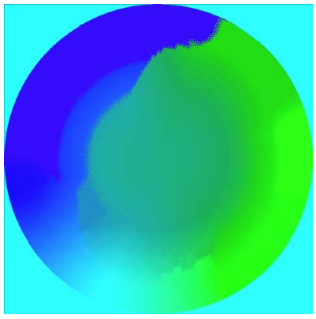

Fig 2. Wheel of hue

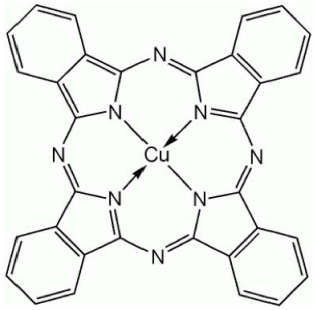

Fig3. Phthalocyanine complex

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