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Application News

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Spectrophotometric Analysis

Evaluating Optical Properties of Diamonds and Natural Gemstones

Diamonds, which captivate the eyes of many people, are either natural or synthetic. Natural diamonds are mined from the earth and synthetic diamonds are artificially made. In recent years, it has become extremely difficult to judge whether a diamond is of natural or synthetic origin by using conventional gemstone appraisal tools and equipment, raising the need for new judgment methods. One such new method utilizes a spectrophotometer.

This article introduces measurements of the reflectance and transmittance spectra of various natural gemstones including diamonds using UV-visible spectrophotometry and Fourier transform infrared spectrophotometry.

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Measuring UV-Vis Reflectance Spectra of Diamonds and Other Natural Gemstones

Fig. 1 shows the two types of diamonds and the natural gemstones of which spectra were measured. Fig. 2 shows a sample set in the sample compartment of the SolidSpec™-3700DUV ("TM" symbol omitted hereafter). The diamond was fixed by fitting the ring portion in a commercially available sponge material and then setting on the sample base. The light beam diameter was set to 1 mm using the light beam aperture mask (accessory) and the area circled in red in Fig. 1 was measured.

Fig. 1 Diamonds and Natural Gemstones that were Measured

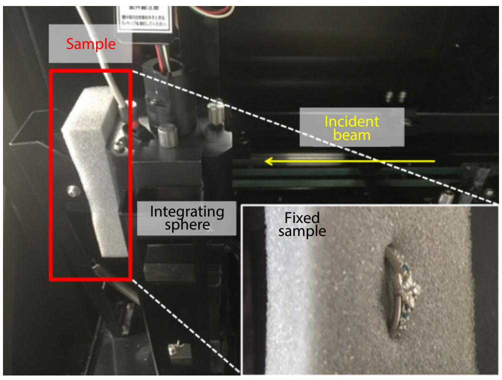

Fig. 2 Inside the Sample Compartment for Measuring a Diamond

Fig. 3 shows the relative diffuse reflectance measurement results (excludes specular reflected light) obtained according to the conditions listed in Table 1. The spectrum from diamond A does not have any prominent peaks, but the spectrum from diamond B shows a peak at 415.2 nm. The optical features of diamonds change depending on the amount of impurities (nitrogen molecules) that are present within. The peak at 415.2 nm in Fig. 3 is considered to indicate the N3 center which comprises three neighboring nitrogen atoms.[1] Since the N3 center is regarded to be proof of a diamond's natural origin, we can assume that diamond A is a synthetic diamond and diamond B is a natural diamond.

Table 1 Measurement Conditions

Instrument Used	: SolidSpec-3700DUV
Wavelength Range	: 400 to 500 nm
Scan Speed	: Very slow
Sampling Interval	: 0.2 nm
Slit Width	: 1.0 nm

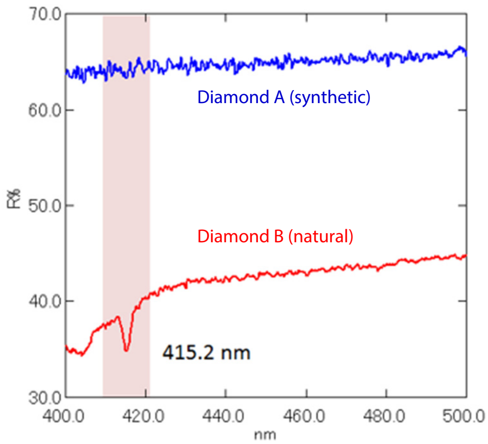

Fig. 3 Reflectance Spectra of Diamonds
Blue: Diamond A (Synthetic), Red: Diamond B (Natural)

We next measured the transmittance or reflectance spectra of the four natural gemstones in Fig. 1. For quartz (rock crystal and amethyst) and fluorite, transmittance spectra were measured because of their high transmittance while for ruby the reflectance spectrum was measured. Table 2 lists the measurement conditions.

Table 2 Measurement Conditions

Instrument Used	: SolidSpec-3700DUV
Wavelength Range	: 300 to 800 nm
Scan Speed	: Medium speed
Sampling Interval	: 1.0 nm
Slit Width	: 5.0 nm

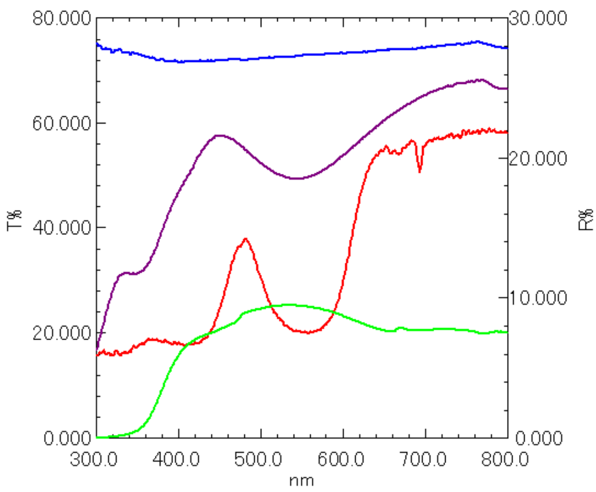

Fig. 4 Transmittance or Reflectance Spectra of Natural Gemstones
Blue: Rock Crystal (%T), Green: Fluorite (%T), Purple: Amethyst (%T), Red: Ruby (%R)

The obtained spectrum shapes differ depending on the color and type of the natural gemstone. Table 3 lists the color values calculated based on the spectra in Fig. 4. Fig. 5 shows the result of drawing these color values using the LabSolutions™ UV-Vis color software and indicates that the obtained color values correspond to the actual color of the natural gemstones.

Table 3 Color Values of Each Sample

Sample	x	y
Rock crystal	0.314	0.330
Amethyst	0.314	0.316
Fluorite	0.314	0.351
Ruby	0.345	0.308

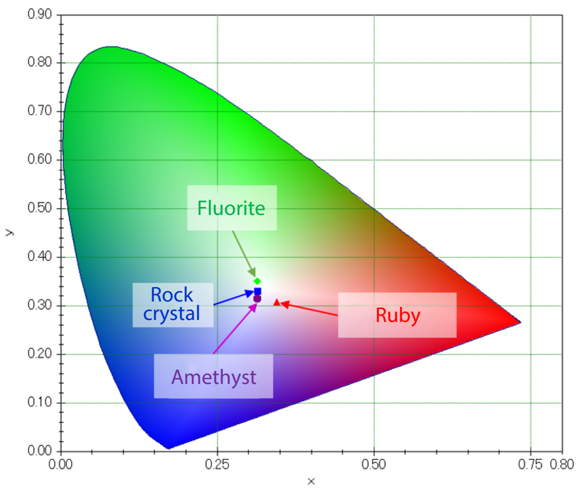

Fig. 5 Calculated Color Values of Various Natural Gemstones
Blue: Rock Crystal, Purple: Amethyst, Green: Fluorite, Red: Ruby

Measurement of the Infrared Spectra of Natural Gemstones

The transmittance spectra of rock crystal and amethyst were measured using the EZClip-13 transmittance measurement accessory shown in Fig. 6. Table 4 lists the measurement conditions. Fig. 7 shows the obtained spectra.

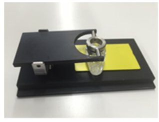

Fig. 6 Sample Set on EZClip-13

Table 4 Measurement Conditions

Instrument Used	:	IRSpirit™-T (KBr window)
Optical resolution	:	4 cm^{-1}
Accumulation Times	:	20
Apodization Function	:	Happ-Genzel
Detector	:	DLATGS

The peak shapes differ between the obtained spectra at about 3400 cm^{-1} in Fig. 7. Amethyst, which gains its purple color due to impurities in quartz, has been reported to have a broad and strong characteristic peak at about 3435 cm^{-1}.[2] These spectra show that the presence of impurities in quartz can be observed by measuring infrared spectra.

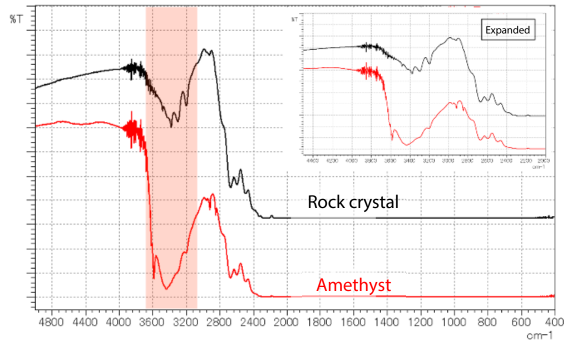

Fig. 7 Infrared Spectra of Quartz
Black: Rock Crystal, Red: Amethyst

Summary

The reflectance and transmittance spectra of various natural gemstones including diamonds were measured using UV-visible spectrophotometry and Fourier transform infrared spectrophotometry. Measurements in the UV-Vis range enabled the judgment of a diamond's natural or synthetic origin. Measurements in the infrared range allowed observation of the presence of impurities in quartz, which are the cause of coloration.

<Acknowledgements>
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<References>
(1) Hiroshi Kitawaki, Characterization of natural and synthetic gem minerals and their applied mineralogy: with special references to compositions, physical properties and fine textures in diamond, 2012
(2) Shoji Kurata, Nondestructive Identification of Synthetic Quartz Crystal Seals Using Spectroscopy
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