Application Note

220-SO-0211

Multiple components analysis by PCA mapping

<Introduction>

Mapping measurement with an IR microscope formally had problems such as difficult sampling and long measurement time. Now, the sample can be treated easily for example by using a tool like SliceMaster and the measurement time can be shortened to less than 1/10 by using a multi-element detector as compared with the traditional mapping system. However, although the mapping measurement itself became easier, much more time is needed for data analysis due to tremendous data points. This report shows some examples of analysis by PCA mapping which enables easier analysis of component distribution from mapping data.

<Experimental>

LCD color monitor shown in Figure 1 was used as a sample with the measurement conditions as follows:

[Measurement conditions]

Detector :Linear array MCT detector Resolution :8 cm^{-1}

Accumulation : 64 times Method : Transmittance

Cassegrain : 16 ×

Measurement time : approx.7 min

Measurement area : 587.5 × 187.5 µm (48 x 16 points)

[Results and discussions]

An observation image of the measured area on LCD color monitor is shown in Figure 1. Each spectrum obtained at the position of A, B and C in Figure 1 is shown in Figure 2. Since the spectra of A, B and C are similar and it is assumed that especially the discrimination of A and C is difficult. The spectra of the main components obtained by the Principle Component Analysis are shown in Figure 3. The spectrum of glass is seen in common among A, B and C in the first main component. The peaks of red pigment from B are observed in the third main component and some very small peaks of A, B and C which are very difficult to be recognized also can be seen in the fifth main component. It is considered that the third and fifth main components represent the specific peaks for each main component and the identification of the components were attempted by plotting the score value of the third and fifth main components shown in Figure 4.

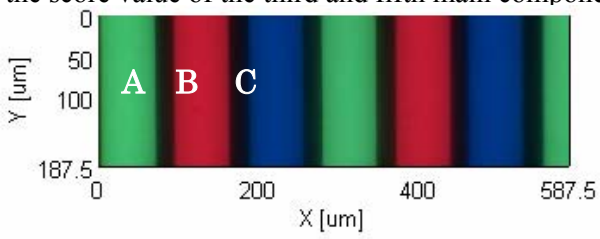

Figure 1. LCD color monitor (Observation image of the measurement area)

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As shown in the area surrounded with dotted line in Figure 4, the plotted score values of the third and fifth main components are eccentrically-located in 3 areas. In PCA mapping, setting color coding of each group from the plot values in the graph in Figure 4 enables to obtain the color distribution diagram shown in Figure 5. In this way, the Principal Component Analysis is considered to be a very useful tool because specific peaks contained in the data can be extracted and compositional distribution is simply figured out by grouping even for the measurement result to be seemingly difficult to identify from the spectra.

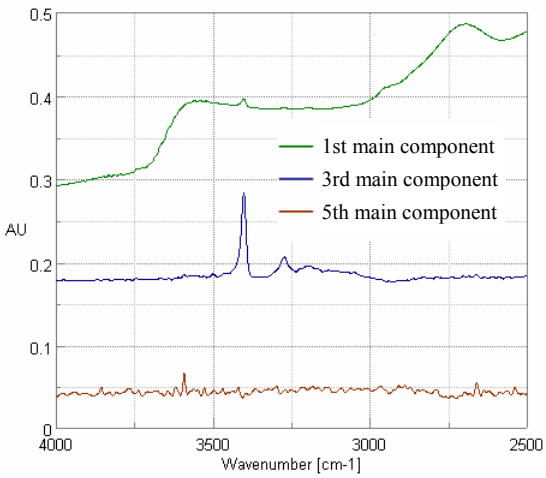

Figure 3. Principal component spectra

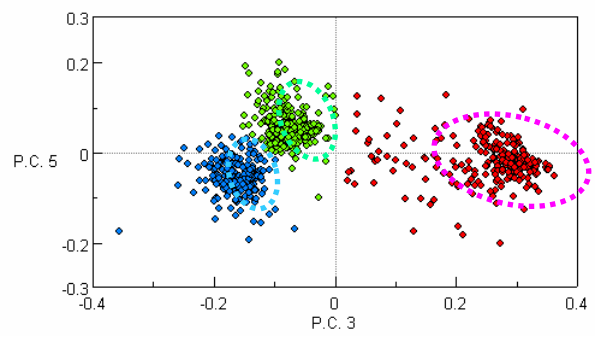

Figure 4. Plot of score values of the third and fifth main components

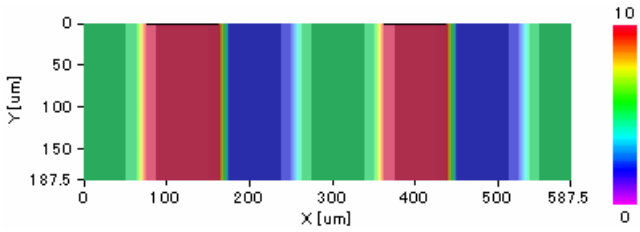

Figure 5. Color distribution diagram of the result by grouping with PCA

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