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Data Spacing of Interferogram for Static Modulation in Fourier Transform Infrared Spectrometer†

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The maximum data spacing of the interferogram for exact spectral information of unknown species was discussed in two dimensional Fourier transform technology for static modulation. We investigated the optimized sampling frequency enough to get the moderate interferogram without superfluous data, based on Nyquist theorem. The Fourier transform infrared spectrometer with a stationary interferometer composed of optical elements creating retardation must use the restrained number of data. The minimum number of data for the static modulated Fourier transform spectrometer was discussed to replace the dynamic modulation in the conventional Fourier transform spectrometers.

Keywords: Fourier transform, Data spacing, Nyquist.

INTRODUCTION

The Fourier transform infrared spectrometer has been used to get the wide and fast acquisition of the spectral information about the unknown species owing to its operational advantages using interferogram[1-3]. It has been commonly referred as a discerning instrument because many toxic and noxious species have the spectral characteristics in the infrared region. Though the theory of Fourier transform spectroscopy has been developed long time ago, many researchers have developed the instrumental technology for more precise and faster investigation about many kinds of materials[4-6]. The possibility of remote sensing is a distinctive merit with a very fast scanning time compared to other spectrometers. Remote monitoring for the inaccessible materials is one of the most important ability of the Fourier transformed spectrometer. The application of the Fourier transformed spectrometer has been extended to many fields of the industrial, military and space surveillance. For the same resolving power and similar instrument size, Fourier transform spectrometers can provide several ten times higher energy gathering capability. Recently it began to be used in common as an atmospheric sounder for monitoring air pollution and clouds movements[7,8].

Some kinds of the Fourier transform spectrometers have already been loaded on the geostationary satellite and are working to provide the monitoring chemical information covered on continents and oceans[9]. However, those Fourier transformed infrared spectrometers are all dynamic modulated types that need a minimal time for the moving optic to scan. It is not suitable for a payload of the low earth orbit satellite, which can get the spectral information at the closer distance from the earth. The conventional Fourier transform spectrometer using dynamic parts of optics to get the optical path difference is not proper to load on a low earth orbit satellite owing to the difficulty to allow even the minimal scanning time to get an interferogram. Another problems for loading on a geostationary satellite are low resolution comparing to that of the dynamic modulated spectrometer, insufficient quantity of the optical input signal due to short exposure time. The key technology for realization of the static modulated Fourier transformed infrared spectrometer is how to generate the optical path difference and how long optical path difference to be acquired. The length of the optical path difference depends on the data spacing or sampling frequency. The static modulated Fourier transform spectrometer has not a moving optic and can get the spectroscopic information at once without scanning[10-12].

In this study, we studied the minimal sampling frequency based on the Nyquist theorem. Two samples of solid and gas phases were used to estimate the maximal data spacing. The absorbance spectra of polystyrene and CO_2 were investigated to compare the spectra of different resolutions. The theoretical

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analysis for the minimal number of data in the specific spectral range and bandwidth was performed for the structural requirement.

RESULTS AND DISCUSSION

Single beam spectra with data spacing

Resolution and data collection time are two important parameters to get the true spectrum of the material. The data collection time concerns how to improve the signal to noise ratio. The longer data collection time provides the more accurate spectrum. In common conventional Fourier transformed spectrometers of dynamic modulated, the longer data collection time means more frequent data scanning. Because the slow scanning for longer data collection time is not proper to get the exact spectral information due to defalcations of mechanical and chemical instabilities in the measuring instrument and the signal source, respectively. Obviously, the larger number of data points in certain spectral range gives the more accurate spectral information of the specimen. However, the infinitesimally small increments of retardation would not be acceptable and therefore, the optimum data points for a certain specimen should be determined according to the material phase.

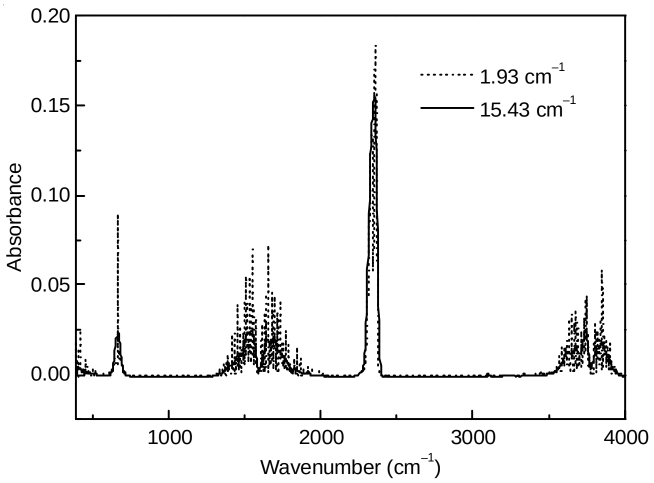

Fig. 1. Absorption spectra of H_2O and CO_2 in two different data spacings

In the measurement of gas phase, the data spacing becomes more effective due to its sharp absorption peaks. Furthermore, the environmental gas noises may disturb the exact measurement for the specimen. Fig. 1 shows the measured absorption spectra of H_2O and CO_2, in two different data spacings of 15.43 cm^{-1} and 1.93 cm^{-1}. The solid line denotes the 15.43 cm^{-1} and the dashed line is for 1.93 cm^{-1}. As shown in Fig. 1, the spectral characteristics of water vapour and CO_2 showed a big difference with data spacing. In gas phases, the higher resolution may be required not to miss the sharp absorption peaks as shown in Fig. 2(a) to 2(d). The lower resolution of 15.43 cm^{-1} is not enough to describe the absorption peak and deep of H_2O and CO_2 around 670 cm^{-1}, 1,600 cm^{-1} and 2,350 cm^{-1} and 3,750 cm^{-1}. Though the higher resolution is effective to execute the exact measurement of a specimen, there is a limitation due to the data capacity to be processed.

In Fig. 2(a), it is not difficult to find the difference between two spectra. The smaller data spacing of 1.93 cm^{-1} shows an absorption peak at 670 cm^{-1} and side lobes that is not in the spectrum of 15.43 cm^{-1} data spacing. Similar phenomenon is in Fig. 2(c) that shows the spectra around 2,350 cm^{-1}. The spectrum of 1.93 cm^{-1} data spacing shows two absorption peaks and one deep, but that of 15.43 cm^{-1} is showing a one blunt peak. Fig. 2(b) and 2(d) have some different problem. The spectrum of 15.43 cm^{-1} is not showing the spectral characteristics completely.

To compare the spectral data in different sampling frequencies of 15.43 cm^{-1} and 1.93 cm^{-1} in three wavelength regions, the absorbance values normalized. Table-1 denotes the values of normalization in two different data spacing.

TABLE-1
NORMALIZED ABSORPTION PROPERTIES
OF TWO SPECTRAL DATA OF SPACING

Band width (cm^{-1})	$\frac{F'(\bar{v})}{F(\bar{v})}$		Difference between 15.43 cm^{-1} and 1.93 cm^{-1} (%)
	15.43 cm^{-1}	1.93 cm^{-1}	
600-750	0.0497	0.0507	2.0 %
2,300-2,400	0.4896	0.4910	0.3 %

Table-1 shows the normalized absorption magnitudes to compare two spectral data of spacing. Two spectral data around 1,600 cm^{-1} and 3,750 cm^{-1} are not presented because Fig. 2(b) and 2(d) have not meaning to compare its normalized absorption values. The higher wavenumber range of 2,300 to 2,400 cm^{-1} showed the smaller difference than that of 600 to 750 cm^{-1}. However, the difference of absorption magnitude is not so large in the range of sensing noise.

Optimum data spacing based on Nyquist theorem

The resolution for the exact measurement should be kept to certain level not to miss any absorption spectral information. The interferograms must be sampled discretely in reasonable number of data points. The problem of how often the interferogram should be sampled can be solved mathematically. The sampling frequency or wavenumber should be greater than or equal to twice the bandpass of the system, which is called Nyquist criterion[13],

$$N_S = \frac{\Delta\sigma}{2\delta}$$

where, $\Delta\sigma = \lambda_{max} - \lambda_{min}$ and δ is data spacing. In order to measure the spectrum of gas specimen, the recommended data spacing was not larger than 1.93 cm^{-1}. The narrow spectral characteristics of CO_2 around 1.573 μm (6,357 cm^{-1}) is possible to measure with the minimal number of data points, because the width of the spectral window is larger than 0.0056 μm (22.5 cm^{-1}). The number of samples can be calculated as following[13].

$$N_S = \frac{\Delta\sigma}{\delta\sigma}$$

where, $\Delta\sigma$ is the width of the spectral narrow filter used to avoid the spectral aliasing and $\delta\sigma$ is the unapodized spectral resolution. This can also be obtained by the relation of

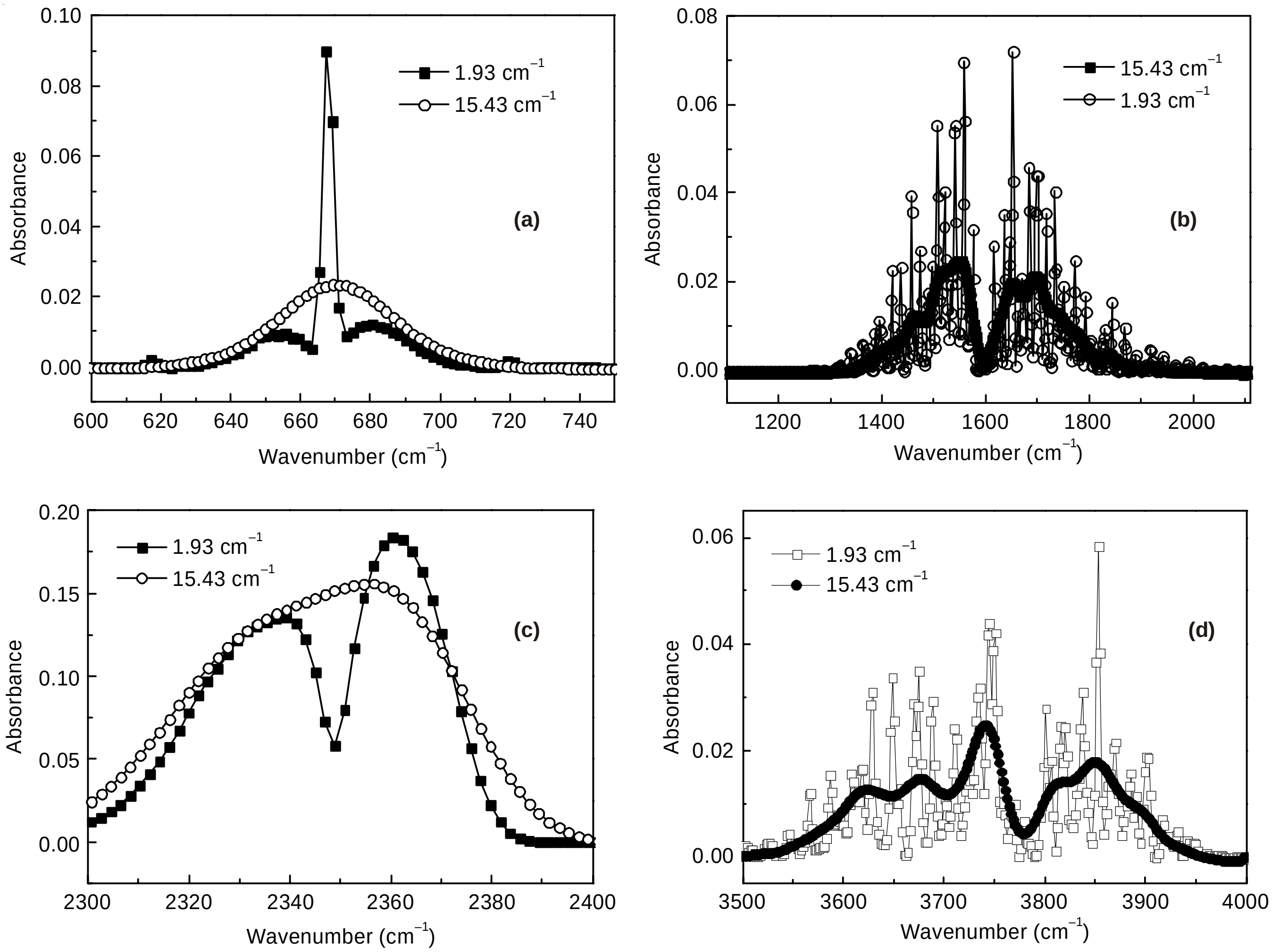

Fig. 2. Absorption spectra of (a) H_2O and (b) CO_2 in different data spacing of 1.93 cm^{-1} and 15.43 cm^{-1}

$$\delta\sigma = \frac{1}{2OPD_{max}}$$

We focused the CO_2 absorption peaks around 1.573 µm, which has the spectral width of about 30 cm^{-1}. If the data spacing were 1.93 cm^{-1} or 0.24 cm^{-1}, the minimal number of data points should be 31 and 249, respectively.

In the design of the static modulated Fourier transformed spectrometer, the number of data points and data spacing are correlated. To detect the absorption peaks of CO_2 around 1.573 µm, the number of data points which have different optical path lengths should be about 250, if the data spacing is 0.24 cm^{-1}. Based on this theoretical assumption, the static modulated Fourier transformed infrared spectrometer can be designed.

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