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Application of NIR and FTIR in Food Analysis

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Abstract: In this paper, we will review the most common spectroscopy technologies for food analysis, their differences and purpose of these differences. Based on the advantages and disadvantages of each technology, we will consider the most appropriate one for every segment of food analysis.

Key words: NIR, spectroscopy, food analysis, chemometrics.

1. Introduction

For more than 20 years, spectroscopy analysis has been used as express method for routine analysis of different food products: from milk to wine, from grain to meat. Due to wide range of different products with different characteristics and properties, it is crucial to find the best appropriate technology to deliver fast, accurate and reliable results with minimum influence on the environment. The two most common technologies for express food analysis are IR spectroscopy with sub-division in NIR (near-infrared) and MIR (mid-infrared). NIR lies in region between 780nm $< \lambda <$ 2,500 nm (12,820-4,000 cm^{-1}) [1] and MIR in region 3000 nm $< \lambda <$ 50,000 nm. Besides, NIR and MIR division there is also such parameter as spectrometer technology which is of great importance with each one has it pros and cons. In this paper, we will review four technologies: Scanning Grating Monochromators, Fixed Grating DDA (Detector Diode Array), FT-NIR and FTIR and kind of applications they are used for [2-4].

2. Materials and Methods

2.1 Scanning Grating

This technology consists of two main compartments: monochromator and rotating grating with a motor.

In fig. 1, light beam from source passes through monochromator, dispersed by grating and transmits (or reflects) the sample to be analyzed. The region of wavelength is selected by rotating of grating [2].

All in all, this technology has advantages and disadvantages respectively as follows:

Advantages:

(1) The best signal/noise ration;

(2) The best wavelength range, particular in the visible region;

(3) The sample heating is very low.

Disadvantages:

(1) A precise internal wavelength standard is required to achieve good wavelength precision;

(2) For instruments with a broad wavelength range, grating anomalies create wavelength regions with rapid intensity variation;

(3) Order sorting filters needed for instruments with a broad wavelength range.

2.2 Fix Grating DDA

Apart from monochomator and grating which is fixed in this technology, there is also one important part-Detector Diode Array. In fig. 2, Light beam from source passes through (or reflects) sample and enters the monochromator, where it is dispersed by grating and passed to diode array detector. The detector performs

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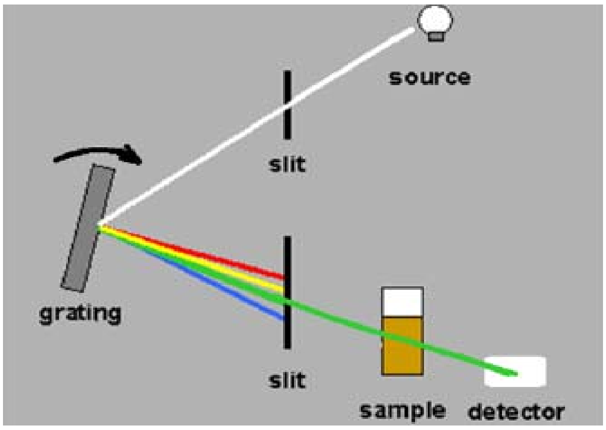

Fig. 1 Scanning grating.

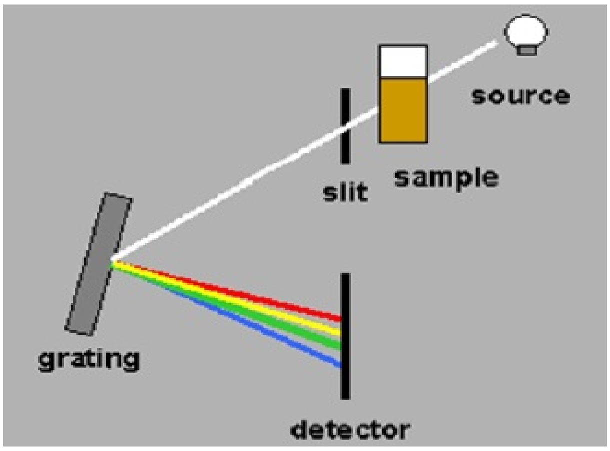

Fig. 2 Fix grating DDA.

reading by means of different pixels and it follows that detector must have a number of pixels required be wavelength range and resolution [2, 5].

All in all, this technology has advantages and disadvantages respectively as follows:

Advantages:

(1) Robust and vibration tolerant design;

(2) Simultaneous measurement of the full spectrum making it tolerant to sample movement.

Disadvantages:

(1) A tradeoff between wavelength range, resolution and signal to noise ratio is needed;

(2) Independent detectors with individual offset and drift properties that need normalization;

(3) Deteriorated signal/noise ratio around the upper limit of the wavelength range for each detector technology. For example, around 1,050nm with Si detector;

(4) Significant sample heating due to broad band sample illumination.

2.3 FT-NIR and FTIR

The only significant difference between FT-NIR and FTIR as the wavelength range the core of technology-Fourier Transformation-is the same. The main part here is interferometer, the unit that creates the IR-interferogram. The IR-signal is emitted from an IR-source. The Laser signal is produced by highly precise and stable laser. In the system, the Beam Splitter, as the name indicates, splits a signal into two: 50% of the signal is reflected, and 50% passes straight through. A fixed mirror (adjustable) simply reflects both the IR- and the laser signal. A Moveable mirror also simply reflects the two signals, but because it moves back and forth in a precisely controlled and parallel manner, the phase of the reflected signal is shifted with the movement. The IR-detector picks up the IR-signal and it is on the surface of the detector that the IR-interferogram is created. The interferogram must be sampled at equal spaced path differences. Information on the path differences is obtained by using a laser as a second source in the interferometer. The Fourier Transformation then transforms the Interferogram into a single beam spectrum [6]. It can be shown clearly in fig. 3.

All in all, this technology has advantages and disadvantages respectively as follows:

Advantages:

(1) The best wavelength axis precision, making spectra easily transferable [7];

(2) Can have high spectral resolution. High resolution is useful for identification of sub-stances but not essential for quantitative measurements;

(3) Resolution can be changed.

Disadvantages:

(1) Lower signal/noise ratio than a monochromator, particularly at short wavelengths. This can be improved by reducing the resolution;

(2) Limited wavelength range in the visible region

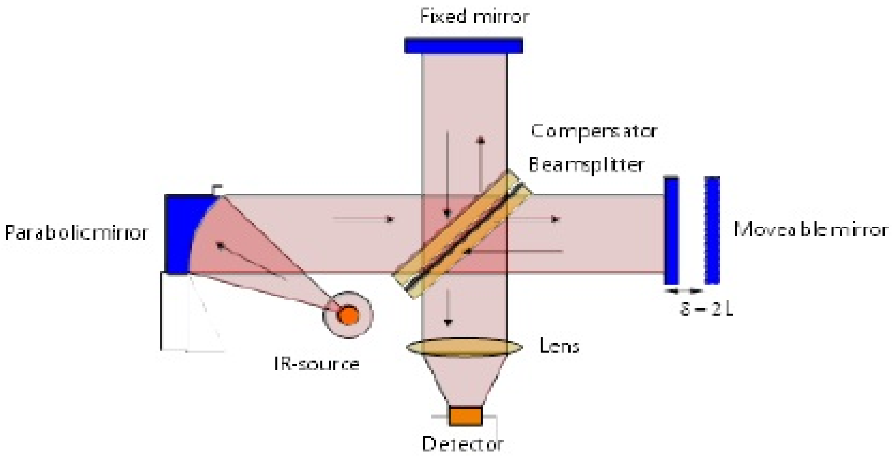

Fig. 3 FT-NIR and FTIR

(below 850 nm);

(3) The most vibration sensitive technology;

(4) Significant sample heating due to broad band sample illumination [5].

3. Results and Discussion

In Food Analysis, it is pretty obvious that we need to separate products whether it is meat or grain, milk or wine, forage or cheese. What is not so obvious is what kind of technology to use? Which one will give us the most?

Due to high and easy-detectable peaks, the resolutions do not play important role in NIR range [8]. It is much more important to have a best signal/noise ration as much as possible.

A fixed grating DDA spectrometer can be used to create robust and vibration-tolerant instruments ideal for use inside production plants. The simultaneous measurement of the full spectrum also makes it tolerant to sample movement. In other words, it is the preferred technology for in-line application. It could be grain or mayonnaise, soya or poultry feed.

For routine analysis of applications in the food and agricultural industries, a scanning grating spectrometer is a proven choice [3]. This includes benchtop compositional analysis of cereal grain, feed, milk powder, ground meat or similar as well as adulteration screening. When using NIR transmission for measuring inhomogeneous grain or meat samples, it is an advantage to use the Short Wave NIR range (850-1,050nm) where the light penetration is good and the premium signal to noise ratio offered by a scanning grating monochromator is essential. A further advantage is that there is little sample heating when the sample is illuminated by a monochromator.

For spectroscopic assignments of pure chemicals where narrow instrument bandwidth is needed, FT-NIR has advantages. The high resolution makes it applicable for pin-pointing substances having narrow absorption bands. The wavelength axis accuracy makes it easy to transfer spectra and the resolution can be adjusted to obtain the best tradeoff between wavelength resolution and signal to noise ratio.

For middle infrared range where peaks are not such high and detectable as in NIR range and difference between them is hard to detect, it becomes important to operate with a high resolution and contrary to FT-NIR, and the signal/noise ratio is much better. In this case, Fourier Transformation provides the best possible results.

4. Conclusions

NIR and FTIR technologies are a great tool to perform qualitive and quantative analysis, but as any tool, we need to clearly understand when and how we can to use them to get the most of it. What is even more important is to remember that these technologies are not rigid. Their core is that calibration models are in constant development. New ones appear every year and old ones are improving. Growth of Chemometrics expands the limits of possibility, and will enable us to do things which seemed incredible just yesterday.

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