

Types of Vibrational Chemical Imaging Instruments

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Commentary

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DESCRIPTION

Chemical imaging (as quantitative – chemical mapping) is the analytical capability to create a visual image of components distribution from simultaneous measurement of spectra and spatial, time information. Hyperspectral imaging measures contiguous spectral bands, as opposed to multispectral imaging which measures spaced spectral bands.

The main idea for chemical imaging, the analyst may choose to take as many data spectrum measured at a particular chemical component in spatial location at time; this is useful for chemical identification and quantification. Alternatively, selecting an image plane at a particular data spectrum (PCA - multivariable data of wavelength, spatial location at time) can map the spatial distribution of sample components, provided that their spectral signatures are different at the selected data spectrum.

Applications

- NIR, IR and Raman chemical imaging is also referred to as hyperspectral, spectroscopic, spectral or multispectral imaging (also see micro spectroscopy).
- Any material that depends on chemical gradients for functionality may be amenable to study by an analytical technique that couples spatial and chemical characterization.
- To efficiently and effectively design and manufacture such materials, the ‘what’ and the ‘where’ must both be measured. The demand for this type of analysis is increasing as manufactured materials become more complex.

Types of vibrational chemical imaging instruments

Mid-infrared chemical imaging: Mid-Infrared (MIR) spectroscopy probes fundamental molecular vibrations, which arise in the spectral range 2,500-25,000 nm. Commercial imaging implementations in the MIR region employ hyperspectral imagers or Fourier Transform Infrared (FT-IR) interferometers, depending on the application.

Near-infrared chemical imaging: The analytical Near Infrared (NIR) region spans the range from 780 nm to 2,500 nm. The absorption bands seen in this spectral range arise from overtones and combination bands of O-H, N-H, C-H and S-H stretching and bending vibrations.

Raman chemical imaging: The Raman shift chemical imaging spectral range spans from approximately 50 to 4,000 cm^{-1} ; the actual spectral range over which a particular Raman measurement is made is a function of the laser excitation frequency. The basic principle behind Raman spectroscopy differs from the MIR and NIR in that the x-axis of the Raman spectrum is measured as a function of energy shift (in cm^{-1}) relative to the frequency of the laser used as the source of radiation.

Fluorescence Imaging: Emission micro spectroscopy is a sensitive technique with excitation and emission ranging from the ultraviolet, visible and NIR regions. As such, it has numerous biomedical, biotechnological and agricultural applications. There are several powerful, highly specific and sensitive fluorescence techniques that are currently in use, or still being developed; among the former are FLIM, FRAP, FRET and FLIM-FRET; among the latter are NIR fluorescence and probe-sensitivity enhanced NIR fluorescence micro spectroscopy and nanospectroscopy techniques.

Data analysis

Data analysis methods for chemical imaging data sets typically employ mathematical algorithms common to single point spectroscopy or to image analysis. The reasoning is that the spectrum acquired by each detector is equivalent to a single point spectrum; therefore pre-processing, chemometrics and pattern recognition techniques are utilized with the similar goal to separate chemical and physical effects and perform a qualitative or quantitative characterization of individual sample components. In the spatial dimension, each chemical image is equivalent to a digital image and standard image analysis and robust statistical analysis can be used for feature extraction.