MULTI-TECHNIQUE DATA TREATMENT FOR MULTI-SPECTRAL IMAGE VISUALISATION

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KEYWORDS
Multi-technique datasets, microprobe techniques, mathematical model, point spread function, automatic matching, multispectral image, visualisation.

ABSTRACT

The 'in situ' investigation of different biological, chemical, physical, and environmental processes often requires the knowledge of these sample characteristics with high - (sub)micro-meter - resolution as a valuable complement to the average bulk information. Different microprobe techniques can meet these requirements and their possible combinations would offer the opportunity of thorough study of a given sample or a scientific problem.
Although some of the existing software packages allow for multivariate statistical treatment of data-sets obtained by a given experimental technique, none of them permits a simultaneous statistical treatment of datasets obtained by different experimental techniques, e.g. by simultaneous scanning μ-XRF (X-ray fluorescence) and μ-XRD (X-ray diffraction), or measured at several set-ups/beamlines/synchrotrons /laboratories (e.g. combined μ-IR and μ-XRF spectroscopy). The goal of this paper is to describe in detail a sequence of operations which can be applied to multi-technique datasets for obtaining a complete set of sample characteristics and to show that at present this can be realised automatically.

INTRODUCTION

The idea of joint analysis of results of polytypic experiments can be found in the literature (Ehmann *et al.* 1993; Bishop et al. 2004, Denecke et al. 2007). Also, commercial software products are available, which support this analysis for certain experimental techniques. Here we refer to CytoSpec as an example. This program is designed specifically for the analysis of vibrational spectroscopic (IR and Raman) imaging data sets. The software permits standard spectral manipulations, such as expansion, smoothing, scaling, normalisation, etc. Univariate methods of analysis consist of various mapping displays of hyperspectral data. The user may select band and integrated intensities, frequencies, intensity ratios, etc. to construct false color maps of the spectral data, which can be considered as slices through the hyperspectral data cube. The multivariate methods of data analysis including Principal Component Analysis (PCA), and unsupervised and supervised methods of Cluster Analysis (HCA), create spectral correlations and maps by including not only one intensity or frequency point of a spectrum, but by utilising the entire spectral information. 3D-Fourier self deconvolution (FSD) is included which allows Fourier self-deconvolution both in two spatial dimensions (x and y) and the spectral/frequency dimensions (z) to be performed at the same time. The method, adapted from the 1-D algorithm described in (Lasch and Naumann 2006), can be applied to enhance the spectral and/or spatial resolution and to increase the image contrast. Despite the numerous advantages, this software package has an essential restriction: the data series (spectra) to be evaluated should be measured with the same equipment.
In this paper we describe a sequence of operations, which could be applied to the evaluation of multi-technique datasets. If this system is built from "black boxes" and each "box" performs a well-defined, independent operation, then the only task to do in order to perform the sequence of operation on the multitechnique data-set is to "connect" these boxes correctly.

Proceedings 22nd European Conference on Modelling and Simulation ©ECMS Loucas S. Louca, Yiorgos Chrysanthou, Zuzana Oplatková, Khalid Al-Begain (Editors)
ISBN: 978-0-9553018-5-8 / ISBN: 978-0-9553018-6-5 (CD)

The following black boxes should be included into this system: “superhigh resolution”, “inverse problem”, “image matching”, and “multispectral visualisation” box. The question of the software interface is omitted from our consideration as we concentrate on the box content itself.

MAIN STEPS

Each measurement technique gives unique information about a sample’s properties. Based on the measured signal formation, a mathematical expression is sought that relates a measured value *S(x,y)* (e.g. a number of quanta) with the sample characteristics *O(x,y)* (e.g. element concentration) for ideal experimental conditions (fine beam etc.). To solve the direct problem means to calculate *S(x,y)*, if *O(x,y)* is known. As a rule, the set-up used for data collection distorts the image by smearing the details. Consequently the so called “apparatus function” or “point spread function” (PSF) has to be taken into account and the model modified through convolution with the PSF. To solve the inverse problem means to reconstruct *O(x,y)* from a measured set of data *S(x,y)* which can be achieved in two steps. The first is known as the PSF deconvolution problem and the second is the reconstruction of *O(x,y)* by solving the equation (Chukalina and Watjen 2001). This operation should be done for each set of data. The next subsequent operation should then be automatic matching of the noisy images of the same sample in the same spectral range with different shifts, orientations and clippings. Finally, the last stage is the calculation of a final image that presents an overview of the images obtained.

Superhigh resolution

The point spread function (PSF) describes the response of an imaging system to a point source or a point object. The degree of spreading (blurring) of a point object is a measure indicating the quality of an imaging system. The point spread function may be independent of the position in the object plane, in which case it is called shift invariant. If the image plane coordinates are linearly related to the object plane coordinates and the PSF is shift-invariant, then the convolution expression describes the image formation

$$S(x_0, y_0) = \int O(x, y) PSF(x - x_0, y - y_0). \quad (1)$$

Where $S(x_0, y_0)$ is the recorded signal and $O(x, y)$ is the signal that we wish to recover. If we know the PSF, or at least know the form of PSF, we can perform deterministic deconvolution. However, if the PSD is not know in advance, then it has to be estimated. In physical measurements, the situation is usually closer to

$$S(x_0, y_0) = \int O(x, y) PSF(x - x_0, y - y_0) + \varepsilon \quad (2)$$

In this case, ε is the noise that has entered the recorded signal. If we assume a noisy signal to be noiseless when we try to make a statistical estimate of PSF, the estimate and consequently also the estimate of O will be incorrect. That is the reason why usual inverse signal filtering is not a good solution. However, if we have at least some knowledge of the type of noise in the data we may be able to improve the estimate of O through Superhigh Resolution Computer-Aided Measuring Systems (SHR CAMS) (Pyt'ev and Chulichkov 1998). The underlying concept of SHR CAMS is a transformation of recorded data into a form they would have if the measurement were performed by an ideal instrument. In order to achieve this, it is necessary to have a complete mathematical model of the data formation process. Since the model will contain errors caused by an approximate description of the real processes, CAMS concepts should incorporates a reliability of the model and a reliability of interpretation. The reliability of the model characterises the consistency of the model for experimental data. The reliability of interpretation characterises the possibility of estimating the object parameters with a guaranteed precision by using the model. The task “from S to O” is known as “Inverse problem. Part I”.

Inverse problem. Part II

This task is reserved for data interpretation. As an example, let us consider the interpretation of m-XRF measurements. A recorded spectrum shows how many quanta of a given energy E were generated in a specimen volume illuminated by a microbeam. Unfortunately, the relation between the number of quanta and the concentration of a given element having this specific fluorescence line is not linear. Several factors should be included into spectrum evaluation and quantification (He and van Espen 1991). To use the data of XRF experiments jointly with diffraction data or with that of some other experimental techniques, it is necessary to know quantitative physical values such as concentration, weight fraction etc. Switching from the data recorded by a receiver to the real physical ones is known as “Inverse problem. Part II”. There are several software packages developed for the XRF spectra interpretation (Espen and He. 1989, Abbott and Adams. 1997, QXAS. 2005). Thus, one image or a set of recorded images represent the input to the box and the image or a set of images, where the physical values are presented, its output.

Automatic image matching

Matching is defined as making or finding the equal or the like of (Heipke 1996). For our task, matching (or registration) can be defined as establishing a correspondence between noisy images of the same sample in the same spectral range with different lateral resolutions, shifts, orientations and clippings. Each of the mentioned factors makes the problem more difficult.

Adding to the complexity is the fact that often different spectral ranges images can have little in common in which case additional knowledge about the images, e.g. the comparison of physical models, might have to be considered.
In general there are two main approaches to image registration: landmark based and intensity based techniques (Brown 1992). While landmark based algorithms rely on the definition of stable corresponding points across the different modalities, intensity based registration utilises all available data to find the best match.

Visualization of multi-spectral images

The final images, which are to be presented to the user, have to include the most important features from the images obtained and processing in previous steps (after convertation the receiver output maps to device-independent data and after matching). An example of a powerful visualisation system is MultiSpec (http://cobweb.ecn.purdue.edu/biehl/MultiSpec) which is a processing system for interactively analysing Earth observational multispectral image data such as that produced by the Landsat series of Earth satellites. New images may be the result of principal component analysis or feature extraction transformations of existing ones, or they may result from the ratio of a linear combination of existing bands divided by a different linear combination of bands. In addition. visualisation algorithms that preserve object boundaries (Nikolaev and Karpenko 2006) will prove useful in this scenario.

CONCLUSIONS

The possibility of obtaining information about diverse sample characteristics such as morphology, crystalline structure, elemental and/or molecular composition and chemical speciation in a non-destructive manner is a general requirement of several research fields such as biology, material science, environmental science, geology, and archaeology. Different microprobe techniques can meet these requirements and their possible combinations would offer the opportunity of a thorough study of a given sample or a scientific problem.
Although existing software packages such as Cytospec (for μ-IR spectroscopy) or AXIL (for X-ray fluorescence), allow for multivariate statistical treatment of data-sets obtained by a given experimental technique, none of them permits a simultaneous statistical treatment of datasets obtained by different experimental techniques (e.g. by simultaneous scanning μ-XRF and μ-X-ray diffraction) or measured at several set-ups/beamlines/synchrotrons/laboratories (e.g. combined μ-IR and μ-XRF spectroscopy). In the paper we have argue the needs for such a system and have highlighted the problems which can arise during system development.

ACKNOWLEDGEMENTS

This work is supported by the RFBR 06-01-22001, 06-02-16117.

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