

Multimodal Visualization and Analysis of Spectral and XCT Data

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ABSTRACT:

An increasing number of industrial applications demand a comprehensive analysis of both structural and chemical composition. Typically, non-destructive testing techniques focus on either structural or chemical characterization but do not deliver both. 3D X-Ray Computed Tomography (XCT) scans are well-suited for determining the internal and external structure of an object at high resolution. The attenuation value it delivers can however be the same or very similar for different materials. For a detailed chemical analysis XCT is therefore combined with spectral characterization techniques such as K-Edge Absorptiometry or X-ray Fluorescence Spectroscopy. In this paper, we are extending a previously introduced framework for visualization and analysis of specimens scanned with these two modalities in multiple ways: For better understanding the dependencies between the spectral energy levels, we propose Spectral Similarity Maps. Spectral Functional Boxplots visualize the statistical distribution of the spectral data. The Spectrum Explorer improves the analysis of specimens of unknown composition. We demonstrate the usefulness of our techniques on several use cases.

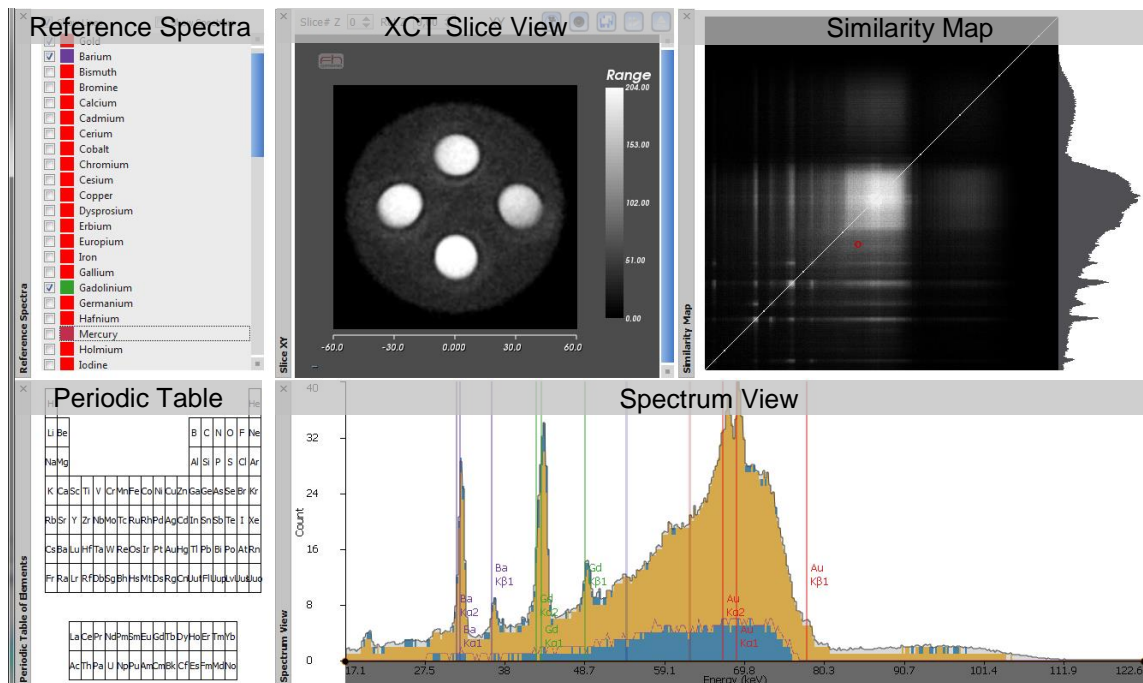


Figure 1. Introduced visualization methods. The upper middle shows a slice view of the XCT data. On the left side is the list of available reference spectra and the periodic table, both used for the interactive exploration of unknown elements. The bottom right shows a Functional Boxplot in the Spectrum View, and the upper right shows the Similarity Map.

1 INTRODUCTION

Industry increasingly relies on non-destructive techniques for detailed product inspection. One modality gaining more and more attention in this area is 3D X-ray Computed Tomography (XCT). According to Heinzl [2], it is fast and can deliver high-resolution scans revealing internal and external structures. At the moment there is a rising demand to also extract a detailed chemical analysis of the scanned object. An XCT device has only limited capabilities in this respect. Spectroscopic methods like X-ray Fluorescence Spectroscopy (XRF) or K-Edge Absorptiometry provide such data, but typically at a lower resolution and with less structural detail when compared to XCT. Therefore data from both modalities are required, so XCT and spectroscopic methods are combined into one device [3].

X-Ray Computed Tomography works by placing a specimen in the direct line between an X-Ray source and a detector. The detector measures the attenuation of the X-Ray when passing through the object. When applying this principle for multiple angles, the resulting 2D absorption images may be reconstructed to retrieve a volumetric 3D representation of the complete object, where each voxel represents the attenuation of the material at this position [4]. In X-Ray Fluorescence Spectroscopy, the detector is placed to the side of the object to measure the characteristic energies of photons emitted when the object is irradiated with X-Rays [5]. The acquisition is repeated from multiple angles to retrieve a 3D representation of the object, where for each voxel a full spectrum is available [6]. K-Edge Absorptiometry in contrast uses a classical CT setup. It retrieves information on the elemental composition by exploiting the connection between attenuation and X-ray photon energy [7].

If a combination of XCT and spectral data is available from the same object, specialized visualization and analysis techniques are required. In our previous work [1] we identified the following three analysis tasks:

- **Global material composition analysis.** The questions to be answered are: Which materials are present in the specimen? How much is there of each material? Where are these located?
- **Local material composition analysis.** The global analysis guides analysts towards regions of interest. Local analysis provides methods for probing their detailed composition and structure.
- **Analysis of unknown and foreign materials.** Specimens of unknown composition are analyzed for their element contents and composition.

We will start with a short introduction into data-visualization methods available so far for such a data combination (chapter 2) which will lead to the motivation for coming up with the InSpectr tool from our previous work [1]. Chapter 3 describes the dataset we used to test our work. We will then give a brief overview on how InSpectr solves the above tasks (chapter 4). Three additional visualization methods for this framework are the main contribution of this paper: The Spectral Functional Boxplot, the Spectral Similarity Map and the Spectrum Explorer. These are explained in detail in chapter 5 where we also outline their usefulness for solving user tasks, and the advantages they provide in comparison to the methods introduced in our previous work. Chapter 6 wraps up with concluding remarks and an outlook on the work we plan to do in the future.

2 RELATED WORK

This work is geared towards the case where XCT and the spectral dataset are consecutively acquired by the same device. The two modalities need to be calibrated and aligned once after the device is assembled, for example by the method proposed by Liu et al. [8]. After that, no further registration of the two datasets is required. For the application of the methods to datasets acquired by different devices, we refer the reader for example to the nonrigid multimodality image registration method by Mattes et al. [9].

In non-destructive testing, material scientists typically start their analysis using software tools like FEI Avizo [10]. These tools provide an abundance of generic visualizations and quantitative analysis for volumetric data, and thus are especially suitable for the XCT data. They do not include analysis tools adapted for our specific combination of datasets. This means that linking between the two datasets and the possibility of combining them in visualization is limited or only possible with extensive in-depth knowledge of the software packages.

Tools for analyzing spectral data like HyperSpy [11], MicroAnalysis Toolkit [12] or PyMca [13] allow the user to analyze single or multiple spectra. They provide sophisticated methods for displaying and processing the spectra, for example regarding element decomposition. They usually do not put them into spatial context and provide no possibility to show other kinds of data alongside the spectral data.

Visualization tools like ParaView [14], VisIt [15] or MeVisLab [16] provide generic visualization and analysis support for a wide range of datasets. They however provide no specialized support for the combination of XCT and spectral data.

There is already a device on the market combining the XCT and XRF modalities. The software shipped with this system provides simple visualization techniques for both datasets [17, 18]. It is limited to showing either separate element maps of the single elements and the XCT data, or an overlaid view of all these maps.

3 DATASET

Tests were conducted on the 2D phantom scanned by Kuang et al. [6] with the prototype of a combined XRF/XCT device at Stanford medical university. It consists of a cylinder filled with water, containing tubular insertions of Barium (Ba), Gadolinium (Gd) and Gold (Au) as well as a mixture of those three in a diluted suspension.

4 INSPECTR

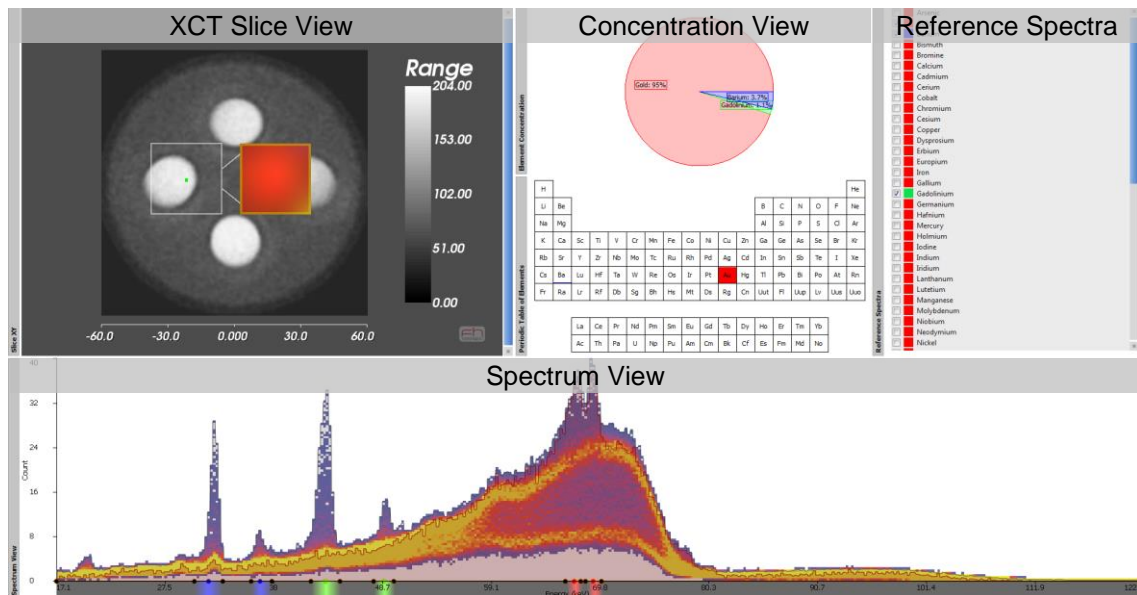


Figure 2. The InSpectr interface contains an XCT slice view, a pie chart and periodic table view showing the element concentration at the current mouse position in the slice view, a reference spectra list and the spectrum view.

InSpectr [1] offers a wide range of views and visualization methods to address all the tasks outlined in the introduction. For the global analysis, the Aggregated Spectrum as well as the Spectra Lines and Spectra Histogram (the latter one being visible in the spectrum view in the lower

part of Figure 2) provide information on which elements are contained in the specimen and in which quantity. The Spectral Color Image (visible in the Magic Lens superimposed on the XCT slice view in the upper left part of Figure 2) and Element Maps in the slicer and the 3D view enable the localization of element occurrences. Local analysis is available from both spectral and XCT side. Selection in the spectrum view highlights the regions with spectra leading through the selected region in the XCT slice. Spectrum and concentration probing link information on the local spectrum and composition to the XCT slice view. The analysis of unknown materials is supported through the ability to display reference spectra in the spectrum view. InSpectr however lacks the ability to statistically analyze the spectral information, to find correlations between peaks and to easily identify unknown elements.

5 NEW VISUALIZATION TECHNIQUES

5.1 Spectral Functional Boxplots

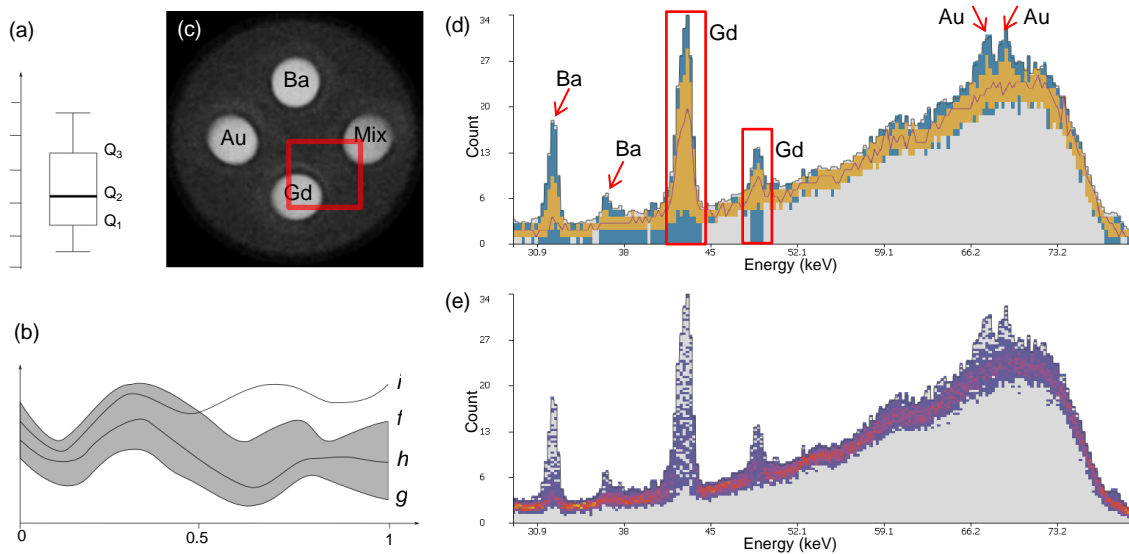


Figure 3. (a) An example for a “classical” boxplot. (b) A function band is spanned by the functions f and g (the grey area). Function h is completely inside the band, function i only between 0 and 0.5, but not between 0.5 and 1. Considering the collection of the four functions, there are six possible function bands of function pairs. The Band Depth for function h would be 5/6, since it is contained in all function bands except the one spanned by f and i . (d) A functional boxplot for the rectangular marked region in (c). The median function is the line in the center (violet), the interquartile range the region around it (yellow), the outer region (blue) is 1.5 times the interquartile range. (e) The spectra histogram for the same region as (d).

The well-known Boxplot (Figure 3a) visualizes five important statistical characteristics of a numerical dataset: The median, first and third quartile and usually minimum and maximum of the non-outlying values. Functional Boxplots, introduced by Sun and Genton [19], extend this concept for collections of functions. They are created by ordering the functions by a metric called band depth. A function band of a set of functions is a region created in a way so that all functions of the set fit into it. As an example, consider the grey area in Figure 3b, it indicates a function band spanned by the functions f and g . For band depth calculation, we create the set S of the function bands from all possible function pairs. The band depth for a function f is the number of bands from S inside of which f fits into over the whole considered interval. The functions are then sorted by decreasing band depth. This creates an ordering from central functions to those lying more outward. The first, most central function in this order is considered as the median function. The interquartile region is determined as the function band of the first fifty percent of the functions ordered by the band depth. For the formal details of the calculation, we refer the reader to the original work on band depth by López-Pintado and Romo [20].

We calculate the band depth for all spectrum functions, and visualize them in a similar way as proposed by Sun and Genton [19], as can be seen in Figure 3. The example in Figure 3d shows the functional boxplot and the histogram of spectra for the same region of interest. The user needs information on the material distribution in this region. The selected region contains a big spot of Gadolinium, and a small spot of a mixture of the elements. In the functional boxplot, the median reaches high up in the Gadolinium peak, indicating a high average concentration. The broad interquartile range indicates a high fluctuation range. At the other peaks, the median remains flat. In contrast to that, the spectra histogram in Figure 3e for the same region shows similar patterns for all the peaks. The shown real-world spectra have low overall-counts and contain a high level of noise, which deteriorates the visualization quality to some extent, but this is similar in both spectra histograms and functional boxplots. In comparison to the spectra histograms, the functional boxplot come with higher computational complexity. For datasets exceeding a few thousand spectra, the accurate computation of the band depth for all spectra is prohibitively expensive. We compensate this by doing an adaptive regular sampling on the set of available function bands during band depth calculation instead of the exhaustive computation.

5.2 Spectrum Explorer

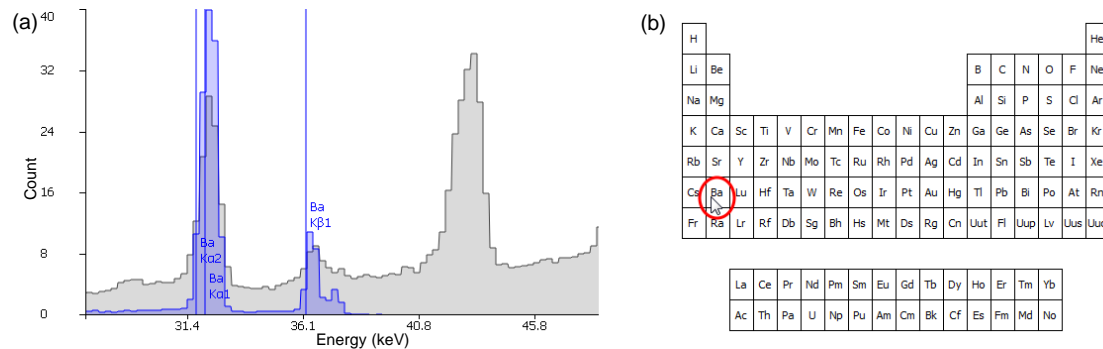


Figure 4. When Spectrum Explorer is active, hovering over the periodic table (b) shows in the spectrum view (a) the reference spectrum and/or the characteristic energy lines for the element under the mouse cursor.

InSpectr provides limited capabilities for exploring unknown spectra. It displays reference spectra when the user selects them in a list. If the precise element contained in a sample is not known, this is a tedious process. In this work we introduce the Spectrum Explorer: While moving the mouse over the periodic table, X-ray spectra from reference measurements [21] and characteristic energy lines denoting the expected positions of the element peaks are overlaid in the spectrum view over any other spectrum visualization. In Figure 4, the user has successfully identified Barium as contained element by matching the reference spectra and energy lines to peaks in the aggregated maximum spectrum.

5.3 Spectral Similarity Maps

Applying the ideas of Bruckner’s and Möller’s Isosurface Similarity Maps [22] to our spectral data, we introduce the Spectral Similarity Map for better understanding the dependencies between the spectral energy levels. The main purpose of the Spectral Similarity Map is to show which parts of the spectrum have strong spatial correlation in the data. For example, if a composite material containing different chemical elements is present in the data, individual spectral peaks of these elements will always appear in the same regions of the dataset. By finding such correlated patterns in the spectrum it is possible to reason about which composite materials or mixtures are present. To achieve this we need to calculate a metric for the similarity between two arbitrary energy levels. For this purpose we consider the values of all voxels for an energy level as a volume, and calculate the similarity of this volume to the volume of every other energy

level through ITK's [24] implementation of the mutual information algorithm as proposed by Viola and Wells [23].

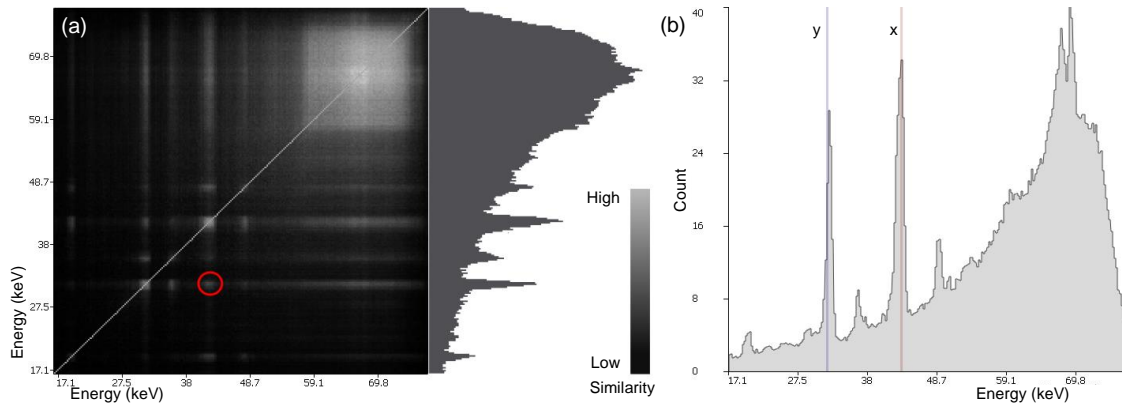


Figure 5. Similarity Map of a spectral dataset (a). The matrix shows the intensity-coded correlation between energy levels; the higher the correlation between the energy levels mapped along both the x- and y-Axes are, the brighter the pixel (x, y). On the right edge of the Similarity Map, an accumulated histogram of similarity is shown. The currently selected energy pair, marked by the red circle, is also highlighted in the spectrum view shown in (b) by the two vertical lines, in the context of the aggregated spectrum. The right line (red) marks the energy selected on the x-Axis, the left one (blue) the energy on the y-Axis.

We then display the similarity using an intensity map image as shown in Figure 5a. The similarity map is symmetric along its diagonal because the mutual information similarity metric is commutative. Mouse Movement over the map area highlights the respective energy levels of the x- and y-Axes in the spectrum view as can be seen in Figure 5b. This helps in identifying the present elements through the Spectrum Explorer. If two peaks show high similarity on the map, this indicates that either these peaks belong to the same element or that the elements they belong to often occur at the same place. If the specimen is not a completely homogeneous mixture of elements, the peaks of the same element will have the highest correlation.

6 CONCLUSION AND FUTURE WORK

In this paper, we introduced three extensions to the InSpectr framework. Functional Boxplots provide insights into the distribution of spectrum functions. Similarity Maps allow the investigation of correlations in the spectral data and can be used in conjunction with the Spectrum Explorer to ease the process of identifying specimen of unknown composition. For the future we are planning to test our extensions with a variety of real and virtual test datasets. We are further planning to extend our cooperation with material scientists to prove the usefulness of our methods in many real-world scenarios.

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