

InSpectr: Multi-Modal Exploration, Visualization, and Analysis of Spectral Data

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Abstract

This paper addresses the increasing demand in industry for methods to analyze and visualize multimodal data involving a spectral modality. Two data modalities are used: high-resolution X-ray computed tomography (XCT) for structural characterization and low-resolution X-ray fluorescence (XRF) spectral data for elemental decomposition. We present InSpectr, an integrated tool for the interactive exploration and visual analysis of multimodal, multiscalar data. The tool has been designed around a set of tasks identified by domain experts in the fields of XCT and XRF. It supports registered single scalar and spectral datasets optionally coupled with element maps and reference spectra. InSpectr is instantiating various linked views for the integration of spatial and non-spatial information to provide insight into an industrial component's structural and material composition: Views with volume renderings of composite and individual 3D element maps visualize global material composition; transfer functions defined directly on the spectral data and overlaid pie-chart glyphs show elemental composition in 2D slice-views; A representative aggregated spectrum and spectra density histograms are introduced to provide a global overview in the spectral view. Spectral magic lenses, spectrum probing and elemental composition probing of points using a pie-chart view and a periodic table view aid the local material composition analysis. Two datasets are investigated to outline the usefulness of the presented techniques: a 3D virtually created phantom with a brass metal alloy and a real-world 2D water phantom with insertions of gold, barium, and gadolinium. Additionally a detailed user evaluation of the results is provided.

Categories and Subject Descriptors (according to ACM CCS): I.3.8 [Computer Graphics]: Applications—

1. Introduction

In state of the art manufacturing, non-destructive testing (NDT) plays an essential role to ensure the quality of new components, not only for prototyping but throughout their complete product lifetime. A widespread modality for industrial non-destructive testing and quality control purposes is 3D X-ray computed tomography (XCT). XCT is capable of high-resolution structural characterizations. It generates single scalar volumetric representations of the inspected object, which consist of local attenuation values. To create these 3D representations a series of 2D penetration images taken throughout a full rotation of the specimen is reconstructed to a 3D volumetric dataset with a scalar value at each

voxel [Hei09]. XCT thus allows the user a highly detailed structural analysis of both external and internal features as well as material interfaces within a single scan. However, in several cases single scalar attenuation values are not sufficient for material decomposition as they produce ambiguous results. Especially for complex, multi-material components attenuation-based XCT is highly error-prone due to artifacts such as beam hardening or streaking artifacts. Regarding non-destructive material analysis X-ray spectrometry methods are increasingly used in industry. Techniques such as X-ray fluorescence (XRF) [BKL*06] or energy-dispersive X-ray spectrometry (EDS or EDX) in electron microscopes [Li02] are found in daily industrial use. The common feature these techniques share is that they are capable of generating spectral information as a vector of response values for different energies or wave lengths. Spectral acquisition modalities

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are attracting an increasing interest in the non-destructive testing and particularly in the XCT community. Recently, the first devices for multi-modal data acquisition combining XCT and XRF have emerged [BSL11, KPB*13], which are capable of generating single scalar and spectral data. Besides the hardware, also the software for the analysis and evaluation is essential in order to facilitate the acceptance of this new technology. Having tools and algorithms that can successfully combine and work with XCT and spectral datasets is thus considered of high importance. Currently, existing software solutions are usually tailored either towards XRF/EDS or towards XCT. These tools are therefore either lacking multi-modal data fusion and visualization functionalities, or they only provide limited visualization capabilities especially for 2D and 3D spectral data. In order to address these shortcomings in existing tools, we have identified these analysis tasks for working with a combination of single scalar and spectral data in close collaboration with XCT and XRF domain experts:

- **Task 1: Global material composition analysis.** Priority one is the identification and localization of all materials present in the inspected object. The user should be able to get an overview of its spectral characteristics. It should also be possible to derive quantitative composition information. Material interfaces in the object have to be determined and visualized. Features of interest as for example traces of certain chemical elements need to be found and classified.
- **Task 2: Local material composition analysis.** After an overview of the global material composition is obtained, a more detailed exploration and analysis in the regions of interest is required. For this task finding and analyzing various defects or irregularities by probing the local elemental composition is done. It should be possible to view spectra at points of interest. Users further want to correlate characteristic peaks with spatial locations in the XCT data.
- **Task 3: Analysis of unknown and foreign materials.** In the areas of research and reverse engineering, the material composition of a specimen is mostly unknown. For this task the detection of elements present in the test specimens including a quantitative analysis is usually of high importance.

In order to address the tasks provided by the domain experts, we developed *InSpectr*, an integrated tool for the exploration and analysis of single scalar data coupled with spectral information. An overview of *InSpectr*'s workflow and its features is depicted in Figure 1. We use registered XCT and X-ray spectrometry datasets as input, which are optionally extended with element maps from the decomposition analysis and/or reference spectra of chemical elements. For a detailed description of input and data preprocessing see Section 3. The process of performing the aforementioned tasks is supported by a large set of visualization techniques: During the visualization and analysis step of the workflow, we

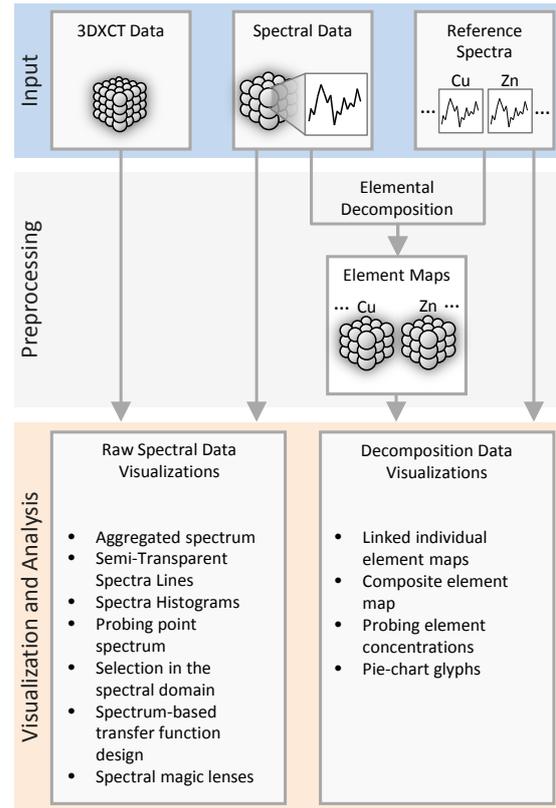


Figure 1: Workflow and features of the *InSpectr* tool.

utilize a set of linked views to provide means of visualizing these multi-modal datasets either in 3D, on 2D slicers, or in a spectral view. For the description of the tool's GUI concepts and individual views see Section 4. The presented visualization methods are divided into two main groups based on the representation of the spectral data. Visualization techniques requiring raw spectral data only are described in Section 5. Visual methods relying on elemental decomposition data are presented in Section 6. We demonstrate use cases suitable for solving the defined tasks by employing combinations of the presented visualization and analysis methods in Section 7. Section 7.1 describes methods for performing Task 1, Section 7.2 is elaborating on methods for Task 2, and Section 7.3 is describing visualization and analysis techniques for Task 3. We evaluated *InSpectr*, using an extended online questionnaire with domain experts in the fields of XCT, XRF, EDS, as well as scientific visualization. Section 8 presents a summary of the evaluation and discusses the results. The core contributions of this work are found in the following aspects:

- A novel integrated tool for visualizing and exploring high resolution single scalar data alongside with low resolution spectral information obtained from the same sample.
- A comprehensive set of visualization techniques allowing

NDT domain experts to perform various tasks of material composition analysis. For this purpose we are utilizing linked views including 3D and 2D views, which are able to convey material composition information as well as the raw spectral information.

- Evaluation based on feedback from domain experts.

2. Related Work

The single scalar and spectral datasets to be used for *InSpectr* are assumed to be generated with the same device. The individual datasets are perfectly aligned and no registration is required. Thus registration techniques are considered as being out of scope for this work. However for further reading we direct the reader to multi modal registration techniques such as Mattes et al.'s non-rigid multimodality image registration [MHV*01] for single scalar data.

Regarding elemental decomposition, dual and multi-energy methods apply the idea of combining two or more attenuation images of the same point of view acquired at different energy ranges of the applied X-ray spectrum. This facilitates extracting information about material composition by calculating the density and atomic number Z , or by providing a new image in a material basis [RD07]. Application areas of these techniques are found in the medical domain [WTW06], as well as airport security [YNC06]. For high precision material decompositions X-ray spectroscopy techniques, such as XRF [BKL*06] and EDS [Li02], are used to provide highly detailed characterizations. Using these kinds of methods at each probed position, a spectrum is generated, consisting of the frequency of each resolved energy bin in the analysis. This spectral information allows revealing characteristic peaks showing the characteristic energies of the materials present in the analyzed specimen. One approach for deriving the material composition from the spectral data is to perform feature extraction by classification. Anderson et al. [AGDJ09] presented a method for range-space segmentation of function field data relying on a specified function distance metric. Clustering methods allow for extracting features of interest such as material areas, but they fail to deliver the quantitative information (e.g., percentages of chemical elements or materials). Therefore various decomposition methods resulting in element maps are commonly applied in spectral imaging. Such methods are presented in works by Solé et al. [SPC*07], Mantouvalou et al. [MMK12], or Schoonjans et al. [SSV*13].

The concept of multiple linked views [Rob07] for integration of spatial and non-spatial information is widely explored in a diverse set of application areas, e.g., medicine [MMH*13], bioinformatics [WRH*09, LSKS10], and geographic information systems [ZTM*13]. Techniques for brushing and linking of function sets are presented in previous works [MGKH07, Kon12]. Information-based registration and fusion of data of different modalities is discussed by Haidacher et al. [Hai11, HBKG08]. A scalable compar-

ative technique for comparing multiple XCT scans using a honey-comb grid is suggested by Malik et al. [MHG10]. In the medical and bio-medical fields, the visualization of large amounts of high-resolution imaging data from various modalities using current advancements in GPU hardware is an important and challenging topic of research [Bey09]. Large and complex datasets in many areas of science and industry induce a high demand in visual analysis tools capable of handling multi-dimensional data, e.g., from simulations or sets of measurements [Pir11]. The concept of magic lenses introduced by Bier et al. [BSP*93] has also proven to be helpful and intuitive in its application to multi-modal data, allowing for easy revealing of features and comparison of modalities.

To our knowledge no tools exist which are capable of visualization and analysis of the multi-modal XRF/XCT data combination. There exist a set of tools for the analysis of spectral data alone, such as HyperSpy [Hyp13], Lispix [Lis13], or pyMCA [SPC*07]. Furthermore, the software for XRF/XCT scanning systems [BSL11] allows the user to overlay colors from an XRF analysis on top of the XCT data as well as assigning colors to the energy ranges to be utilized in the volume rendering. The state of the art technique for visualizing material composition based on XRF data is using 2D element maps, and 2D composite element maps [KPB*13]. In the field of scientific visualization there exist many works on multi-modal and multi-material analysis and visualization. Software tools for scientific visualization as Paraview [Hen04] or VisIt [CBW*11] currently provide no solution tailored to the combination of XRF and XCT modalities. ParaView provides a framework for the development of such solutions supporting the VTK and ITK open source libraries. VisIt supports working with energy groups. Our tool is implemented within iAnalyse - a custom framework using VTK and ITK. It contains additional tools and instruments for convenient work with 3DXCT data and workflows. With *InSpectr* we aim to extend state of the art techniques combining XCT and spectral data, by linking both modalities in one seamless visual analysis workflow. We believe that currently no such tool exists in the field of non-destructive testing.

3. Input Data and Preprocessing

InSpectr requires a single scalar dataset and a spectral dataset as input. Both are acquired from the same specimen (Figure 1 (input)), and must be registered to each other. The single scalar dataset may be generated from any 2D or 3D NDT modality providing at each spatial position a single data value. In our application cases we use 2D and 3D XCT scans, which are represented as volumetric data with one scalar attenuation value per voxel. Possible modalities for the spectral data include XRF or EDS. The spectral data typically consists of a single spectrum per voxel. Such a spectrum provides counts of photons for defined energy bins as

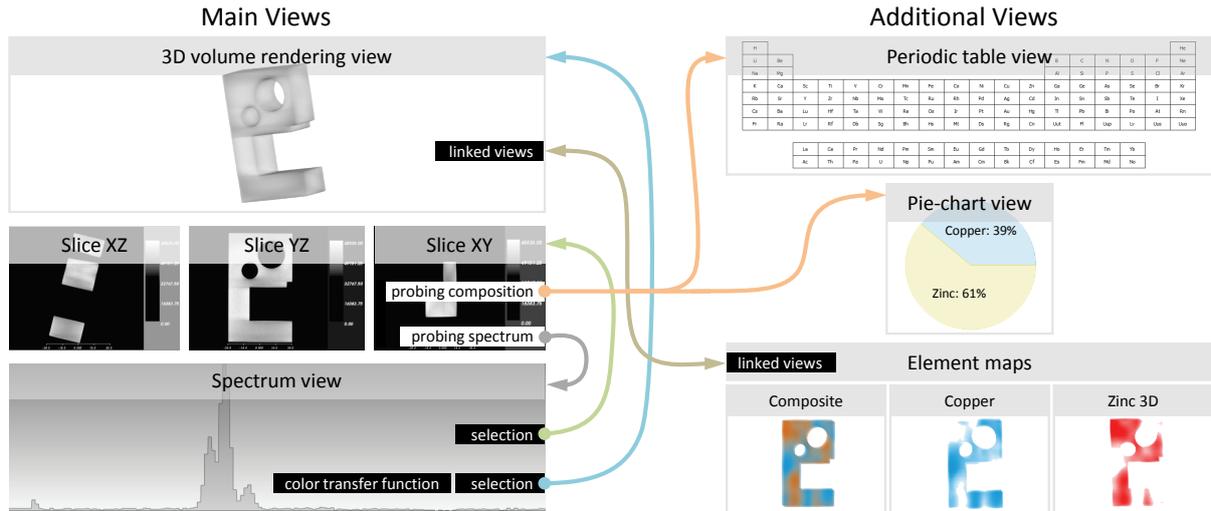


Figure 2: Schematic of InSpectr's interface and the interactions between the available views

measured in the scan of a specimen. The spectrum of an element has one or several characteristic peaks at specific energy levels, corresponding to the photons emitted from different types of transitions between specific electron orbitals. The spectral data is in most cases generated on a lower resolution than the scalar data. This is due to limitations of the spectral method itself, such as maximal penetration depth or self-absorption at low fluorescence energies in case of XRF. Furthermore, not all spectral measurement methods are able to penetrate the specimen. Even for those which allow sub-surface data generation, the penetration depth will vary with the type of measured material, and usually is only in the micrometer range. The methods proposed in this paper therefore fit best for small specimens, down to the micro- and nanometer scale.

Many of the analysis and visualization techniques discussed in this paper allow for comparisons to the reference spectra. Ideally each reference spectrum is derived from a scan of a specimen consisting of a single material. However, also simulated spectra or spectra available from any databases may be used.

3.1. Preprocessing

Depending on the manufacturer and used software, some preprocessing may be required to extract the spectral data from the XRF/EDS scans. Such preprocessing may vary between different devices. The preparation of the spectral data is out of scope of this work (similar to the preprocessing or reconstruction techniques of XCT scans).

Some of our visualization techniques require element maps. In an element map, the scalar value at each voxel represents the concentration of an element in the specimen at

that position. As an approximation, the spectrum of a composite material can be seen as a weighted sum of the spectra of the elements it consists of. We can therefore calculate element maps by fitting a weighted sum of the reference spectra for each voxel spectrum. The resulting weights correspond to the concentration of the respective elements. We used least linear squares fitting to generate element maps for our test samples. For the alloy test dataset, we performed the decomposition concerning the two contained elements. The spectral dataset is a $125 \times 125 \times 112$ volume, where each voxel contains array of 512 energy bins. The decomposition calculation took about 85 seconds when running on an Intel Core i7-2600 with 16GB RAM. Designing an optimal decomposition method, which considers physical phenomena of X-ray propagation and attenuation, is out of the scope of this work. Third-party decompositions can be applied externally and subsequently imported into InSpectr.

3.2. Test Specimens

We used one scan of a real-world 2D phantom and one virtually created dataset to demonstrate our techniques. The 2D water phantom dataset was measured by Kuang et al. [KPB*13]. It contains conical tube insertions of Gold (Au), Gadolinium (Gd) and Barium (Ba) and a mixture of these three elements, suspended in water. Furthermore, we used spectra from the literature [LN13] to create a test object containing a varying combination of Copper and Zinc, emulating a brass alloy with varying quality.

4. Introduction to InSpectr's Interface

InSpectr provides various views, each giving different visualizations and different aspects of the specimen. A schematic

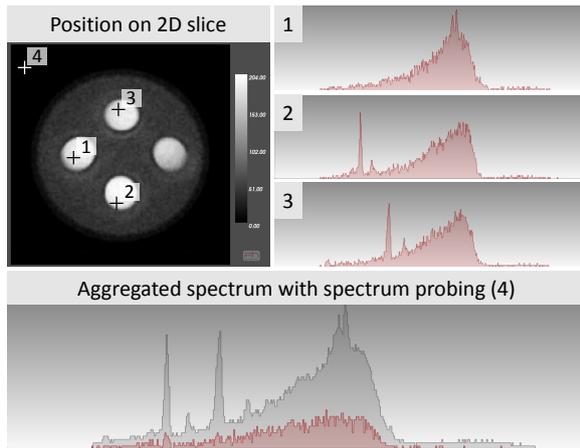


Figure 3: Aggregated spectrum view using the maximum values of voxel spectra. In 1-3, individual voxel spectra probed on a 2D slice are shown. The image at the bottom shows spectrum at point 4 together with the aggregated spectrum in gray.

overview of InSpectr’s basic interaction possibilities is shown in Figure 2. 3D and slicer views visualize the XCT data using color- and opacity transfer functions, typical for volume rendering of scalar data. Using spectral data, or an element decomposition, the slicer and 3D renderer can be enhanced with color-coded overlays of the spectral data. *Element maps* show the volume-rendered result of elemental decomposition. A *spectrum view* shows a variety of visualizations related to energy spectra. Using a list of *reference spectra* it is possible to compare them between each other. *Pie-chart* and *periodic table* views show element concentrations. Through linked updates, these views provide information on a local and a global level.

5. Spectrum-Based Visualizations

The first group of techniques is working with raw spectral data (see Figure 1). The key view used by the spectrum-based visualization techniques is the spectral view. It shows the measured energy spectrum with photon energies on the horizontal axis and photon counts on the vertical axis. We provide an aggregated spectrum view (see Section 5.1) with semi-transparent spectra lines or spectra histograms (Section 5.2) for a better spectral overview. Then probing a point’s spectrum (Section 5.3) can be used to study a specimen’s points of interest in more detail. For bringing characteristic peaks in the spectral view into correlation with their spatial locations in the XCT data we propose selections in the spectral domain (Section 5.4), spectrum-based transfer functions (Section 5.5) and spectral magic lenses (Section 5.6).

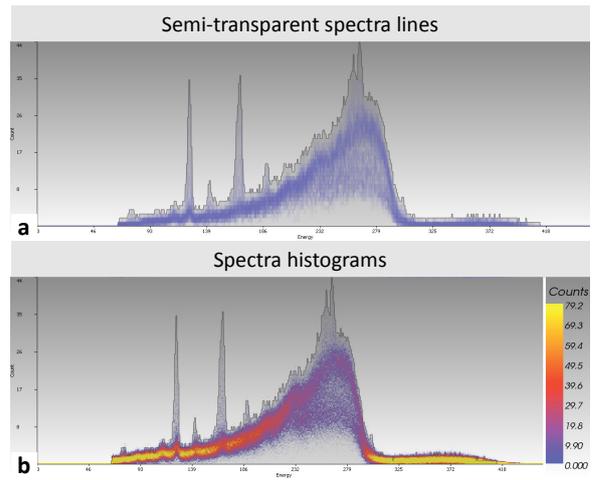


Figure 4: Semi-transparent spectra lines (a) and spectra histograms (b). The aggregated spectrum is shown in gray in the background.

5.1. Aggregated Spectrum View

To achieve an overview of the spectral characteristics of a specimen, an aggregation of the individual spectra is performed with the constraint of preserving features such as peaks, their positions, and heights. To compute an aggregated spectrum for the inspected object we iterate over the individual spectra at each voxel and calculate the maximum value for each given energy bin. Figure 3 shows the individual spectra at the selected positions 1, 2, 3 and the corresponding aggregated maximum spectrum below. The individual peaks are well preserved in this representation. We also calculate an average spectrum, which provides an overview of occurrence rates.

5.2. Semi-Transparent Spectra Lines and Spectra Histograms

The aggregated spectrum provides a concise overview of the spectral properties for the entire dataset. With it, it is possible to aggregate and display the characteristic energy peaks for all the elements present in the data. It, however, lacks the information about the quantities of certain values which histograms typically provide for scalar data. For example using the histogram of the scalar volume, it is possible to estimate the proportion of regions with similar scalar values through the heights of corresponding peaks. For the aggregated spectrum such a shape analysis is not possible since it provides an overview of higher-dimensional data (1D energy spectra instead of scalars). To additionally visualize the distribution of individual voxels’ spectra in the spectral view color coding can be used. We present two techniques depicting spectrum distribution information on the spectral view: semi-transparent spectra lines and spectra histograms (Fig-

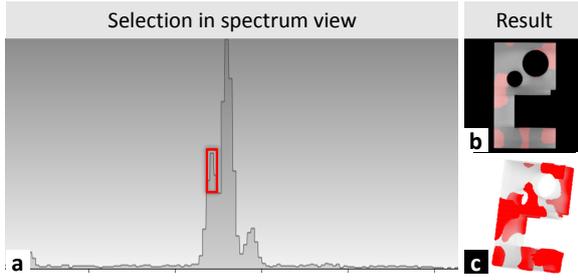


Figure 5: Selection specified in the spectral view (a) and the selection results on the 2D slice (b) and in the 3D view (c).

ure 4). The semi-transparent spectra lines visualization (Figure 4a) is displaying blue regions which are formed by semi-transparent lines, one for each voxel spectrum. The spectra histograms visualization (Figure 4b) is building a histogram for each energy bin. Such a histogram contains information about the number of individual spectra with similar photon counts for a given energy value. A color map is applied to visualize the resulting histograms. The user can interactively adjust the color mapping windowing or select another color map.

5.3. Probing Voxel Spectrum

For interactive spectrum exploration, InSpectr employs voxel spectrum probing. When the user is hovering a mouse cursor over the 2D slice view, the spectrum for a voxel under the cursor is displayed in red (see Figure 3). The aggregated voxel spectrum can be shown for context. Such an interactive workflow allows for fast and uninterrupted probing voxels' spectra and comparing them between each other in the context of the aggregated spectrum. The spectral view allows visualizing the voxel spectrum in the context of all other spectral visualizations proposed in this paper.

5.4. Selection in the Spectral Domain

Another analysis technique of InSpectr is the selection in the spectral domain, depicted in Figure 5. The user can specify one or more rectangular filter regions in the spectrum. Two selection modes are available: *logical AND* or *logical OR*. For *logical AND* only those voxels are selected which have a spectrum that passes through *all* specified filter regions. For *logical OR* those voxels are selected which have a spectrum that passes through *any* specified filter region. After determining the voxels selected by the given filter, InSpectr will highlight all those voxels in the slicer and 3D renderer, as can be seen in Figure 5.

5.5. Spectrum-Based RGB Color Transfer Function

We present a method for defining an RGB color transfer function directly on the spectrum. The color of each voxel

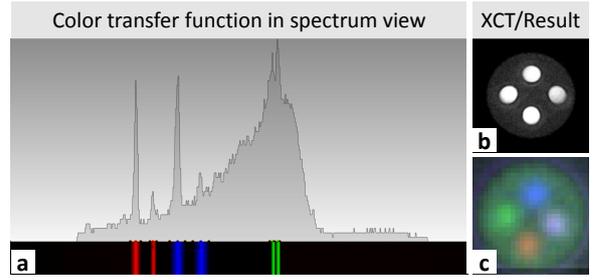


Figure 6: Color transfer function defined in the spectral view (a), XCT slice (b), and resulting spectral color image (c).

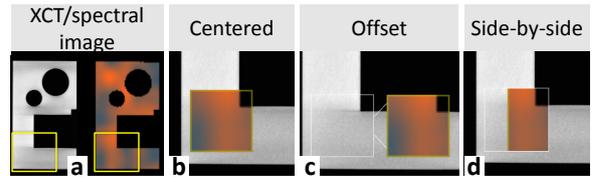


Figure 7: The XCT data and the corresponding spectral color image (a). Spectral magic lenses: centered (b), with offset (c), and side-by-side (d).

is determined by combining the intensity of a peak in the spectrum with the RGB color assigned to that position:

$$C(x, y, z) = \sum_{i=1}^n S(x, y, z, i) * L(i) \quad (1)$$

n is the number of discrete energy levels in the spectrum; $L(i)$ denotes the color as defined in the transfer function on the spectral view for energy bin i (a vector representing the RGB values), and $S(x, y, z, i)$ a function delivering the count at energy bin i in the energy spectrum of the voxel (x, y, z) . In order to assure that accumulated colors fit into the RGB color space, we normalize them by the maximum color component value of all the voxels' accumulated colors. The resulting color for each pixel is dominated by the energy levels with high counts and high color intensity. Calculating the color for each voxel in the spectral data according to equation 1 results in the spectral color image. This can be overlaid directly on the 2D slicer images as can be seen in Figure 6.

5.6. Spectral Magic Lenses

InSpectr uses spectral magic lenses for showing the spectral color image in the 2D slice (see Figure 7). Depending on the use case, there are three possible operating modes: The image can be directly overlaid on the original image in the region of interest (Figure 7b), allowing to alternatively view the scalar and the spectral data. The spectral image can also be shown with an offset to the side (Figure 7c), to allow concurrent viewing of scalar and spectral data for better compa-

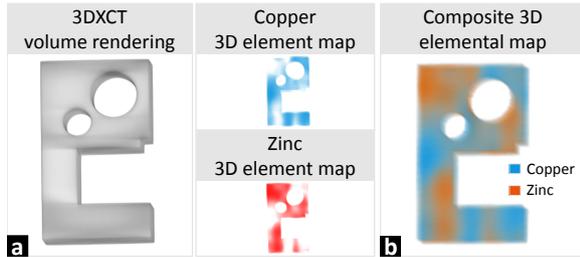


Figure 8: (a) Linked 3DXCT volume rendering and individual 3D element maps; (b) Composite 3D element map for TP09 specimen showing copper and zinc concentrations.

rability. Where close proximity between scalar and spectral data is required for the comparison, the magic lenses can also be split up between showing the original image and the spectral color image (Figure 7d).

6. Decomposition-Based Visualizations

If a quantitative analysis of the elemental composition is required, spectral data is hard to analyze and interpret. For this purpose, an elemental decomposition is performed, resulting in element maps. Element maps represent the concentration distributions for individual chemical elements present in the data. We provide element map views linked to the view showing the XCT data to facilitate an interactive exploration process. Complementary composite 3D element maps assist the material interfaces identification (Section 6.1). For deriving local composition information we propose the probing of element concentrations (Section 6.2). Finally, pie-chart glyphs (Section 6.3) provide local quantitative composition information combined with the global element distributions in the context of the XCT scan.

6.1. Linked Individual Element Maps and Composite Element Map

To assist interactive exploration and analysis of a specimen's elemental composition we utilize linked 3D individual element maps (Figure 8a). Element maps corresponding to each chemical element of the specimen are shown in a separate 3D view using volume rendering. A color for each element can be assigned by the user. The 3D view with XCT data provides a high-resolution context and is used for user interactions. The camera is shared between the XCT 3D view and 3D element map views and all the views are updated correspondingly when an interaction occurs. This guarantees that the user will always see linked views with the same view angle and camera position. This allows uninterrupted exploration and visual analysis workflow. The fact that all element maps are always co-registered and provide information in the context of the 3DXCT data also simplifies comparisons between the views. The identification of different materials'

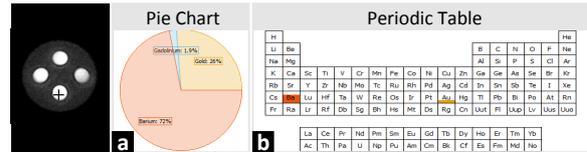


Figure 9: Elemental composition at selected voxel, visualized in the pie-chart view (a) and in the periodic table view (b)

interfaces can often be challenging when individual element maps are shown separately. For such cases a composite 3D element map can be employed (Figure 8b). Multi-channel volume rendering is used to combine individual 3D element maps with different colors. At the moment the visualization toolkit used for volume rendering limits us to combining a maximum of up to four such maps. The resulting visualization is able to show regions with individual elemental distributions as well as regions containing multiple elements. The material interfaces can be seen as regions with color transitions.

6.2. Probing Element Concentrations

Using the element map, InSpectr visualizes the detailed distribution percentages via a pie-chart view for a voxel marked in the slicer (see Figure 9). Another visualization of a voxel's element concentrations is available through a periodic table view. Here, the elements at the marked position are highlighted by drawing a color bar inside each element's box, with the height of the bar varying with the concentration of the element: The higher the concentration of an element, the higher will be the corresponding bar.

6.3. Pie-Chart Glyphs

InSpectr provides pie-chart glyphs, which show regional concentration information and are overlaid over the XCT data, as depicted in Figure 10. The concentrations shown in these glyphs are calculated by resampling the element maps to a resolution so that in the resulting image one voxel corresponds to one glyph. The glyph therefore shows the average concentration of elements for the region beneath the glyph. The glyph's resolution, opacity, and spacing can be varied to support different analysis goals. Note that element concentrations do not always sum to 100%, as element maps are not necessarily normalized, or possibly not all elements are considered during elemental decomposition.

7. Use Cases of Task Solving

For each of the tasks defined by the domain experts, there are several visualization and analysis techniques available in InSpectr. We present those use cases in detail and show

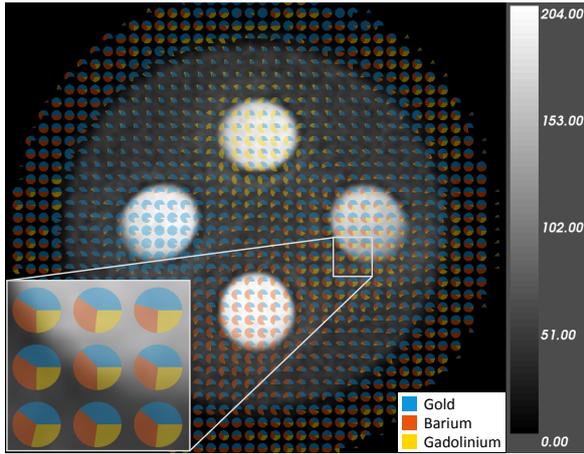


Figure 10: Pie-chart glyphs

which of our methods can be applied for which task. Our two test specimens are used to demonstrate concrete examples.

7.1. Task 1: Global Material Composition Analysis

For a quick first overview on the spectral data, InSpectr provides aggregated spectra, showing the maximum or average spectrum, as can be seen in Figure 3. The maximum spectrum preserves local peaks, thus giving a first insight into characteristic peaks throughout the specimen while the average spectrum considers the occurrence rate of the different energy bins. Spectra histograms and semi-transparent spectral lines visualize patterns in the spectra. They are emphasizing energy counts occurring with higher frequency than others, thus allowing an insight into elemental concentrations. With such representations it is now possible for the user to visually identify an outline of the most commonly appearing individual spectra and even clusters corresponding to different chemical elements. For example, in Figure 4, the lower arc corresponds to air surrounding the specimen and the higher arc to water in which the cylindrical inclusions are placed. The inclusions themselves correspond to weakly colored regions inside energy peaks in the aggregated spectrum. This indicates that the volumes of the inclusions are relatively small compared to the total volume. If elemental decomposition data is available, pie-chart glyphs can be overlaid on the scalar data in the slicers. Figure 10 highlights a spot where the glyphs indicate a roughly equal distribution of Gold, Barium and Gadolinium. Through linked individual 3D and 2D element maps (see Figure 8) InSpectr enables understanding of where material interfaces are located. Orienting the individual element maps in the same way as the 3D renderer for the scalar data allows easy referencing between the modalities.

7.2. Task 2: Local Material Composition Analysis

The selection in the spectral domain (see Figure 5) provides an intuitive way of finding local concentrations of materials of interest. The characteristic peaks of the desired elements can be determined via reference spectra. Those peaks can then be selected in the spectrum, causing InSpectr to mark regions having voxel spectra traversing the marked region. This method can be applied for finding both high and low element concentrations. By combining multiple selections in the spectrum also a specific combination of elements can easily be found in the specimen. This allows us to determine areas which have an elemental concentration deviating from the expected distribution, e.g., defects in the specimen. Also traces of an element are easily localized by selecting this element's characteristic peak in the aggregated spectrum. To further classify a defect or irregularity, the user can display the spectrum for a chosen voxel for gaining an initial insight into the local element composition. InSpectr's spectral view displays the voxel spectrum in the context of other spectral functions. As Figure 3 shows, local peaks can be mapped against peaks in the aggregated spectrum. For studying local element concentrations, InSpectr provides the magic lens showing the spectral color image. This image gives an intuitive representation of which color-marked characteristic peaks in the spectrum appear where in the current region of interest. By displaying the color-mapped spectral and scalar data directly next to each other, the magic lens is especially useful for the comparison of the two modalities. This allows us to gain further insights into any kind of irregularity, as for example the uneven distribution of copper and zinc visible in Figure 7. Furthermore, InSpectr enables the user to show the local elemental distribution in the familiar environment of a periodic table. Even more detailed information on the exact percentage of each element prevalent at the selected voxel can be obtained through the pie-chart view, which is showing the local elemental distribution (see Figure 9).

7.3. Task 3: Analysis of Unknown and Foreign Materials

When analyzing specimen with an unknown material composition, InSpectr allows us to identify characteristic peaks in the aggregated spectrum. By comparing these peaks to reference spectra, the domain expert can match the peaks and thereby determine elements contained in the specimen. The spectrum selection technique can be applied for a broad range of use cases. It is useful for searching for high element concentrations by selecting an element's characteristic peak, no matter if it is already known which element it is. By combining selections it is possible to, for example, select all places where a high concentration of specific single elements is found. Furthermore, the concentration of a combination of several elements can be selected. The user can then compare the spectral data to the corresponding regions in the scalar data. Also useful in the context of unknown materials is the

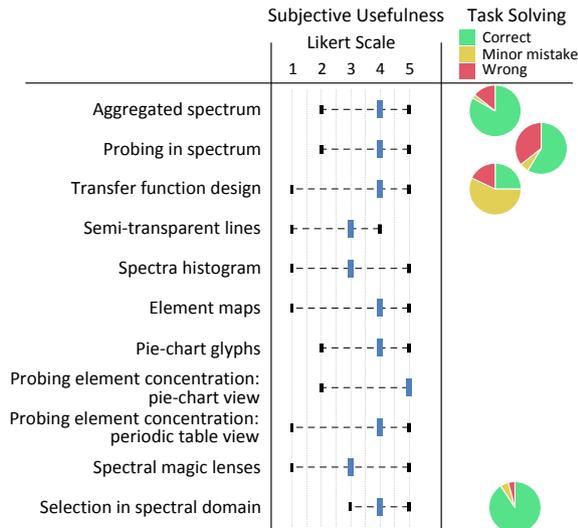


Figure 11: Evaluation results: subjective usefulness and task solving ability are evaluated for the presented techniques.

definition of a color transfer function on the spectrum, as can be seen in Figure 6. The figure clearly indicates three differently colored regions corresponding to peaks in the spectrum, and one appearing to be a combination of these.

8. Evaluation Results

In order to evaluate InSpectr, we presented an online questionnaire to the domain experts in fields of XCT, XRF, EDS, and scientific visualization. A total number of 14 domain experts participated in the evaluation. Illustrations and video demonstrations of the visualization techniques proposed in this paper were presented. Two types of actions were required from the participants: First, the users were requested to perform several analysis tasks or to provide the interpretations using the given visualizations. Additionally subjective feedback about the usefulness of the visualizations for the tasks at hand was collected. Figure 11 provides a graphical representation of the obtained evaluation results. The general feedback was very positive. Our user study clearly shows that the proven method of probing in the spectrum is a useful tool. However, probing the element concentration via pie-chart views and the selection in the spectral domain were perceived as even more useful. The low error rate seen in the study also suggests that the selection in the spectrum is very intuitive. Pie-chart glyphs, the aggregated spectrum and transfer function design on the spectrum were also seen as having high potential. The spectral magic lens and element maps were considered useful as well. Semi-transparent lines were not received so well. The similar spectra histograms did a bit better, but were also only slightly on the side of use-

ful techniques. We believe that the used specimen were not well-suited for these techniques. We expect to see a better applicability for them for different specimens in the future.

The feedback from the domain experts hinted at the possible limited usefulness of the spectra histograms. It was noted that high counts were mainly visible in regions of Compton scatter. One further remark was the impression that the color blending used for example in the spectral transfer function would work well for up to four different materials, but could be problematic for more. In contrast to that, the pie-chart view was perceived to be suitable for a much higher number of materials. A suggestion for an improvement of the periodic table visualization was to fade out materials not included in the specimen. For the spectral view the usage of filters was proposed to remove noise and to accentuate peaks better. From our observation and also from the results of the user study, we conclude that visualizations as simple as pie-charts provide a very intuitive and quick way of conveying composition information. One reason is probably the familiarity of such charts. The periodic table view performed worse here as it suffers from the drawback that only a very small region of the whole visualization is conveying the important information about elemental composition.

9. Conclusion and Future Work

We presented InSpectr, a tool enabling the interactive exploration, analysis, and visualization of the XCT scan data coupled with the spectroscopic modality. First, together with the domain experts we formulated three important analysis and visualization tasks: global material composition analysis, local material composition analysis, and analysis of unknown and foreign materials. Then we demonstrated how visualization techniques based on the raw spectra and on the elemental decomposition data support the user in performing these tasks. By applying the presented visualization methods the experts are now able to obtain important insights on the material composition in an integrated uninterrupted fashion. We provided a user evaluation of InSpectr functionality which indicates high usefulness and importance of such methods. In future work we intend to integrate advanced material decomposition methods and implement additional views providing information on the material elemental concentrations, mass, and volume.

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