On the use of spectral tomography for rock characterization

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INTRODUCTION

X-ray micro-computed tomography (micro-CT) enables non-invasive 3D imaging of materials. Herein, the contrast mechanism depends both on the material-specific X-ray attenuation coefficient and the density. Many combinations yield a similar attenuation and therefore distinguishing them is challenging. Recently, laboratory-based spectral X-ray micro-computed tomography (sp-CT) has emerged as a promising solution, sensitive to both material composition and density, thus offering improved material identification in a non-invasive way.

MATERIALS AND METHODS

Sp-CT and micro-CT both employ a polychromatic X-ray source. The difference between both is that sp-CT detects the energy of each individual photon impinging on the detector, unlike micro-CT, which only detects the cumulated energy deposited by the X-ray beam. Sp-CT therefore records the shape of the polychromatic spectrum, where micro-CT records the integral of that spectrum. At each energy level, the relationship between intensity before and after passing through a material is described by the Beer-Lambert law. By exploiting this law, Sp-CT yields an energy-dependent attenuation coefficient in each reconstructed voxel. By comparing the shape of this reconstructed signal to the real material- and density-specific quantity, information about the composition and density can be obtained.

Every element has a characteristic absorption edge at a specific energy and can be identified if the energy associated to this absorption edge is in the practical energy range of the spectral detector at hand. If absorption edges fall outside the detectable range, it is still possible to detect chemical or density variations with the following strategy: two energy intervals (at low and high energy ranges) are selected, and for each voxel, the averaged mass attenuation coefficients over both energy ranges are calculated. The mass attenuation coefficient averaged at low energy is then plotted against the mass attenuation coefficient averaged at high energy, resulting in a 2D multi-energy histogram. All voxels with the same chemical composition cluster along a line in this 2D multi-energy histogram. The slope of this line is thus dependent on the chemical composition only, while the distance from the origin highlights variations in density solely.

We acquired scans with a Tescan UniTOM XL Spectral (DMEX, Pau, France) in conventional (micro-CT) and spectral (sp-CT) imaging mode. This instrument features a polychromatic X-ray source and two detectors: a 16-bit flat panel detector (2856 x 2856 pixels) for micro-CT, and a linear CdTe detector (384x1 pixels) for sp-CT. The detectable energy range of the spectral detector ranges from 20 keV up to 160 keV in 1keV intervals, permitting the identification of elements with atomic number greater than 42 via their absorption edge [1-2]. Micro-CT data were reconstructed with Panthera (v 1.4.3.16), while sp-CT data were processed using the Spectral Suite (v2.1, Tescan).

RESULTS AND CONCLUSION

Here, we present two examples, demonstrating the effectiveness and added value of sp-CT compared to micro-CT for the discrimination between light-element bearing components (atomic number lower than 42, for which the absorption edge is outside of the detectable energy range of the spectral detector). The employed data analysis approach is based on the 2D multi-energy histogram.

The first example [3] presents the spectral signatures of carbonate rock-forming minerals, namely calcite, magnesian calcite, dolomite, and magnesite, composed of light elements (Ca, Mg, C and O), and which have a different proportion of magnesium. The slopes of the separate clusters of each mineral on a 2D multi-energy

histogram (figure 1) correlate with the mineral composition, serving as a diagnostic feature. A linear regression of the histogram slope against $MgCO_3$ mol. % (obtained by XRD powder analysis) in the sample yields a strong correlation. This result indicates that spectral CT can be used to track for replacement reactions such as dolomitization, even on the same sample (time lapse spectral CT).

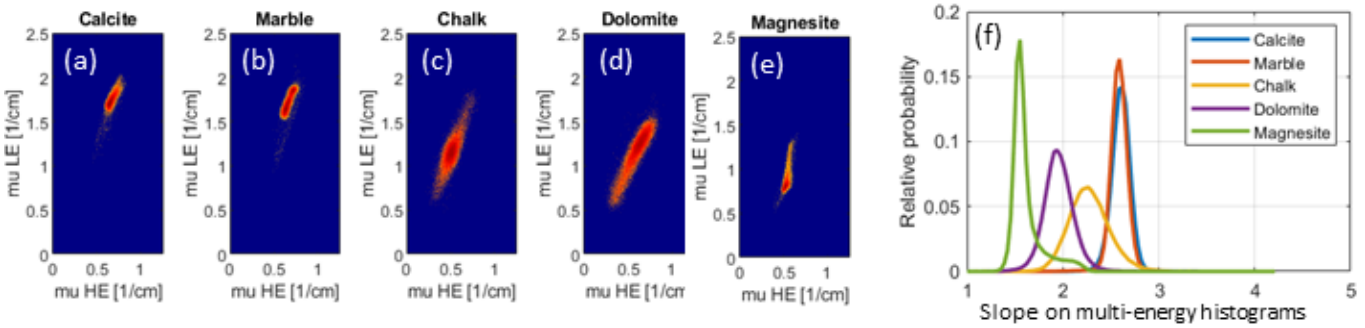

Figure 1: 2D multi-energy histograms obtain of with results of (a) calcite ($CaCO_3$); (b) marble ($CaCO_3$); (c) chalk ($(Mg,Ca)CO_3$); (d) dolomite ($MgCa(CO_3)_2$); (e) magnesite($MgCO_3$) and (f) their corresponding histogram of slopes. The low-energy (LE) range (30-55 keV) and high-energy (HE) range (90-120 keV) were used to construct the multi-energy histograms.

In a second example [4], we performed a blind test on a natural monzo-diorite sample with a more complex mineralogy. Without a-priori information, classical micro-CT allowed to discriminate between four phases. Sp-CT data represented in the 2D multi-energy histogram enabled the differentiation between nine clusters, based on subtle variations in chemical composition and density. Independent micro-Raman and SEM-EDX analysis confirmed that these distinct clusters correspond to different mineral phases. The improved discriminating potential of sp-CT is essential when studying source rocks, for example in the context of natural hydrogen exploration, where the pyroxene-amphibole transition or fayalite-serpentine transition are potential markers for hydrogen production.

The examples demonstrate that sp-CT can be used for visualizing, monitoring, and quantifying mineral phases and/or chemical reactions non-invasively, even in absence of detectable absorption edges. This opens up perspectives on the use of spectral tomography in several applications in geosciences.

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