

## On the relevance of spectral tomography for material characterization

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### 1. Introduction

X-ray micro computed tomography (micro-CT) is a key technique for non-destructive 3D imaging of materials. Image formation in micro-CT is based on the X-ray attenuating properties of material phases, that are dependent on their density and composition. However, many combinations of composition and density yield a similar linear attenuation coefficient, and distinguishing them is therefore challenging by means of conventional micro-CT. Recently, laboratory-based spectral X-ray micro-computed tomography (sp-CT) has been proposed. This technique is sensitive to the material composition, and therefore holds the promise of improved material discrimination, or even material identification. Here, we present different cases in which sp-CT is effective.

### 2. Materials and Methods

Sp-CT was performed using a Tescan UniTOM XL Spectral (DMEX, Pau, France). This instrument is equipped with a polychromatic X-ray source and two detectors, namely a 16 bit flat panel detector for conventional CT imaging and a linear CdTe-detector for Spectral imaging. Sp-CT was conducted on one slice, operating the X-ray source at 160 keV and 20W with 800 spectral projections over 360°. The reconstructed linear attenuation coefficient at each voxel is comprised of 140 equidistant energy bins of 1 keV between 20 and 160 keV. The data were reconstructed and analyzed using the Polydet suite (v3, from Tescan).

### 3. Results and discussion

We provide several examples demonstrating the effectiveness and added value of sp-CT compared to micro-CT:

➤ *Detection of a chemical element not visualized by conventional micro-CT.* Palladium (Pd) impregnation in a carbon gel cylinder was analyzed using sp-CT. The spectra show a distinct peak corresponding to the K-edge of Pd in the external part of the cylinder with decreasing amplitude towards the sample core. This corresponds to a decrease of Pd concentration from the surface to the center (Figure 1).

➤ *Possibility to distinguish minerals with similar chemical composition.* Gabbro may contain minerals

such as amphibole and pyroxene. Both are silicates contain the same minerals, but, in different proportions. This difference does not provide contrast in conventional micro-CT, while the spectra obtained with sp-CT show small differences at low energies, allowing for phase discrimination.

➤ *Evidence of density changes in a rock by using sp-CT.* Micro-CT images of coin-shaped oil shale samples show mainly two phases with a slightly different reconstructed attenuation. While micro-CT enables phase discrimination, it ignores the origin of the attenuation change. Sp-CT analysis highlights density changes for an otherwise stable chemical composition.

➤ *Monitoring of chemical reactions involving both compositional and density changes.* The gradual dolomitization of a chalk cylinder is monitored by micro-CT and sp-CT. The dolomitization front is visible on both image modalities but sp-images demonstrate that the chemical reaction involves both density and chemical composition changes not discriminated by micro-CT.

Independent analyses from SEM, EDS, infrared and Raman spectroscopy confirmed the given results.

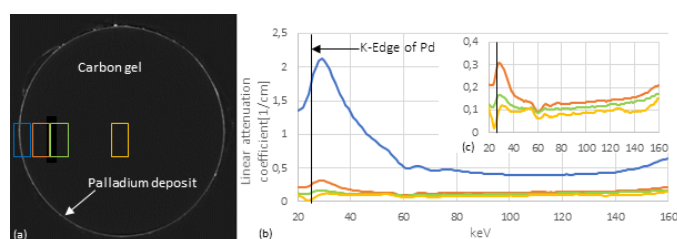


Figure 1 (a) Sp-CT slice of a carbon gel cylinder (5mm diameter) after impregnation with Palladium. (b) Mean spectra obtained at the positions indicated in (a). (c) Zoom of (b). Mean spectra in blue, orange and green clearly show peaks corresponding to the K-Edge of Palladium, unlike the mean spectrum in yellow.

### 4. Conclusions

Unlike conventional micro-CT, sp-CT is able to identify elements with a high atomic number and to detect and distinguish between compositional and density changes in materials. These results reveal the relevant position of laboratory sp-CT in material science and earth sciences.

### 5. Acknowledgements

The projects were supported by E2S UPPA hub Newpores, Nouvelle-Aquitaine Region, the "France 2030" investment (ANR-16-IDEX-0002), CNRS (TellUs and PEPS), Carnot ISIFOR, ERC grant No 850853.