New developments in 3D LA-ICP-MS imaging: Advanced alignment and analysis techniques

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Compositional imaging by laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) has largely focussed on high-resolution two dimensional images. In the past few years however, there has been increasing interest in 3D applications for LA-ICP-MS imaging from a range of disciplines. There are a variety of approaches available for 3D imaging, each with certain advantages and disadvantages. Here we present a comparison of three approaches applied to a single sample in order to highlight the most appropriate use of each. We then examine the 3D volume reconstruction approach, which is possibly the most complex, in more detail.

The 3D volume reconstruction approach builds an 'image stack' which requires some form of alignment post-processing. We recommend the pyramidal voxel registration technique as it is less likely to be affected by user bias, and has no requirement for common landmarks between images. This technique allows for alignment based on a single channel, or a composite channel, which may produce more accurate alignments overall for some samples.

Once the image is aligned and the data reduced to concentration values, there is the issue of how best to represent multiple channels for 3D datasets. We present one solution to this problem via a multi-criteria voxel-gram. We also address the problem of how best to examine both the spatial and compositional distribution of 3D datasets with a murine brain example dataset from the field of neuroscience. We have developed an *n*-dimensional 3D fuzzy clustering approach to identify natural compositional clustering within our example dataset, the spatial distribution of which can then be visually inspected via the voxel-gram.

This process paves the way for combined image sources to provide additional information to our datasets and to help improve the accuracy of our LA-ICP-MS results.