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Introduction

For 3D microstructure characterization in material science, X-ray tomography is an attractive non-destructive technique¹. To exploit this technique a series of data processing steps are required in the tomography pipeline. Each of these steps can be performed using a variety of methods and each step will introduce errors and uncertainty to different degrees that will propagate through the pipeline. This means that it is challenging to assign meaningful error bars to the extracted parameters², which in turn limits the strength of the conclusions that can be drawn based on the measurements. In this project, we look into the uncertainty in the extracted material parameters, aiming for a better understanding of how errors propagate through the pipeline of tomography and affect the accuracy of the final result.

The tomography pipeline

Problem

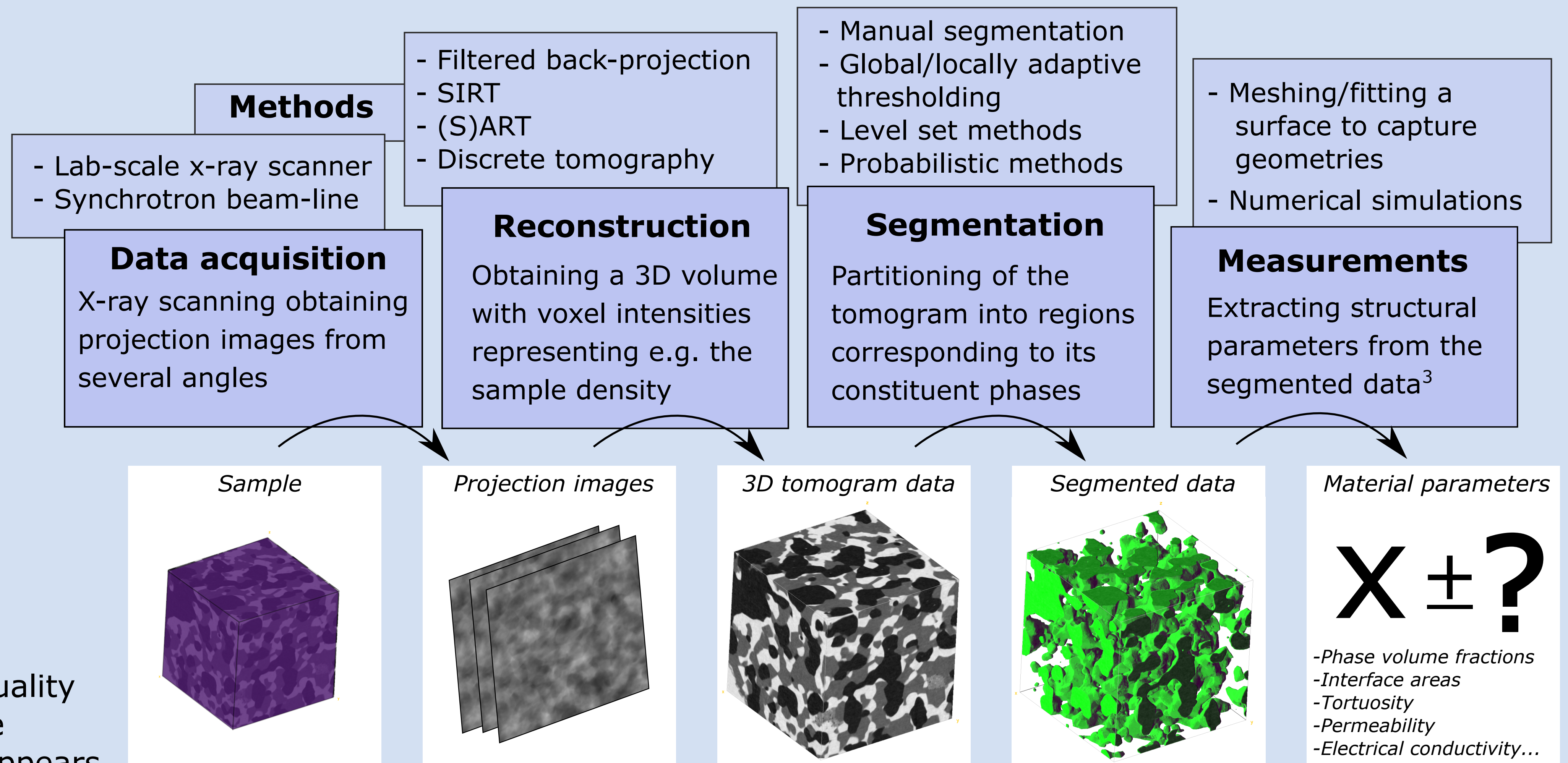
Each of the steps in the pipeline can be performed using a variety of methods. Errors and uncertainty is introduced that will propagate through the pipeline. This makes it challenging to assign meaningful error bars to the extracted material parameters².

A theory that models and propagates errors and uncertainty through the analysis pipeline is crucially needed.

Initial investigations will focus on the segmentation and measurement steps.

Issues with the current approach

When measuring material parameters in the segmented data, the accuracy depends on the quality of the segmentation. Often, the evaluation of the segmentation quality is based on what visually appears to be correct⁴. This is problematic because it introduces an operator bias, can be time consuming and makes the results difficult to reproduce. For huge data sets like tomography time series, manually assessing the segmentation result is no longer feasible. Moreover, the lack of a ground truth makes it challenging to assess the uncertainty.

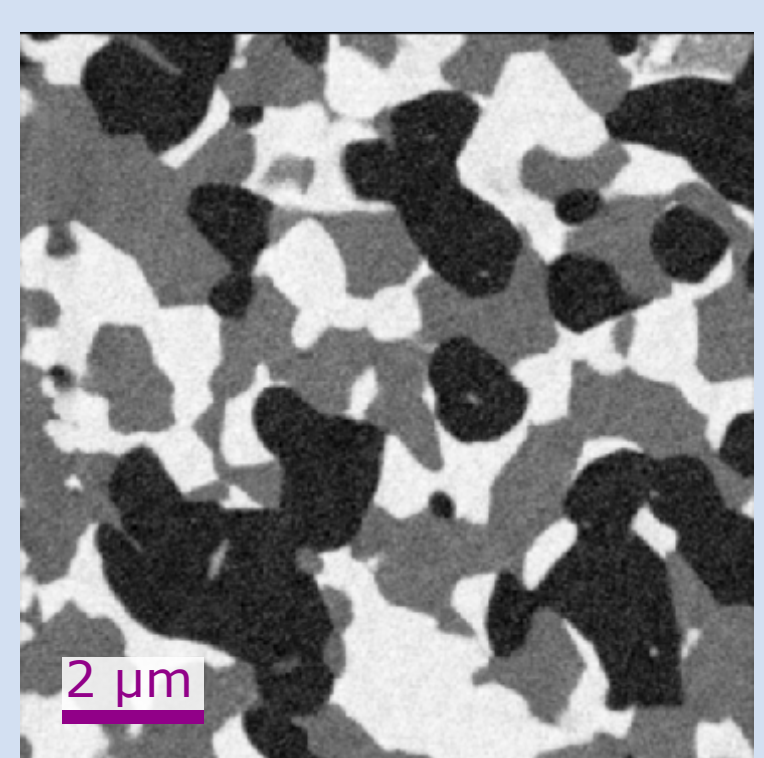


Measurements through physical modelling

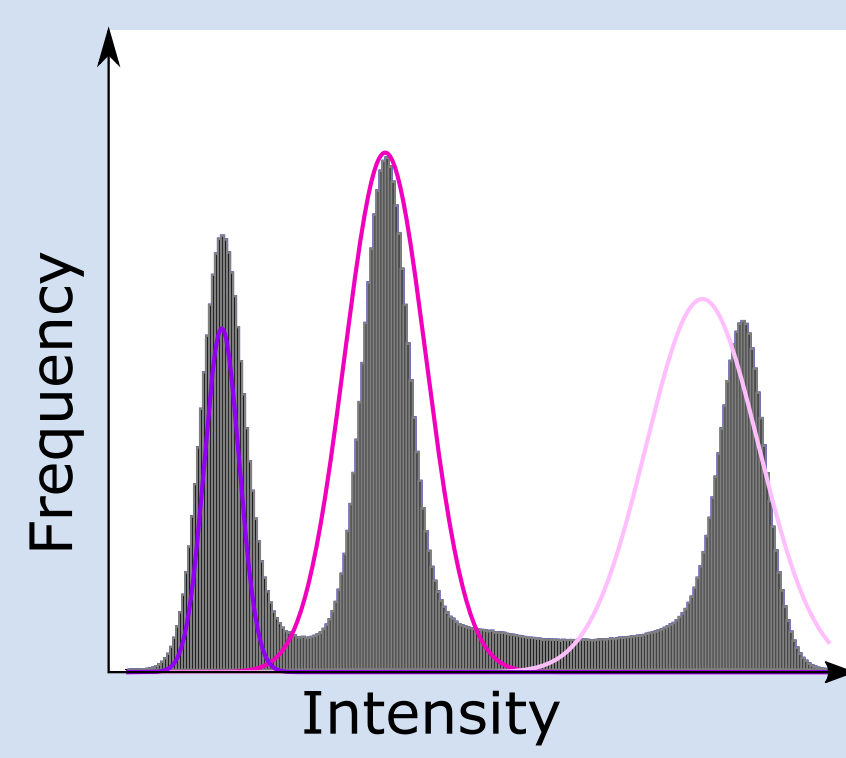
Our approach will be to extract material parameters by fitting a model directly to the tomogram data, skipping the segmentation step. This introduces a consistency check, as it provides a way to evaluate the quality of the segmentation result, regardless of the choice of method, by directly comparing the results of the two different measurement approaches.

A basic physical model

We illustrate the type of physical models the project seeks to develop on 3D image data of a solid oxide fuel cell obtained by ptychographic nano-tomography².



Fuel cell tomogram data



1D intensity histogram with fitted GMM

In this example, we know that our tomogram data contains three different materials. A simple approach would assume that all the image intensities could be described by three different intensities with added Gaussian noise. This corresponds to a Gaussian mixture model (GMM) with three components. If this model fits the data well we would expect to be able to extract the phase fractions and noise levels from the fitted model parameters. However, as can be seen from the histogram, the model fits this data poorly. What is missing from this very simple model are the interfaces between phases. The next step is therefore to include interfaces and other physical parameters in the intensity distribution model.

Further work

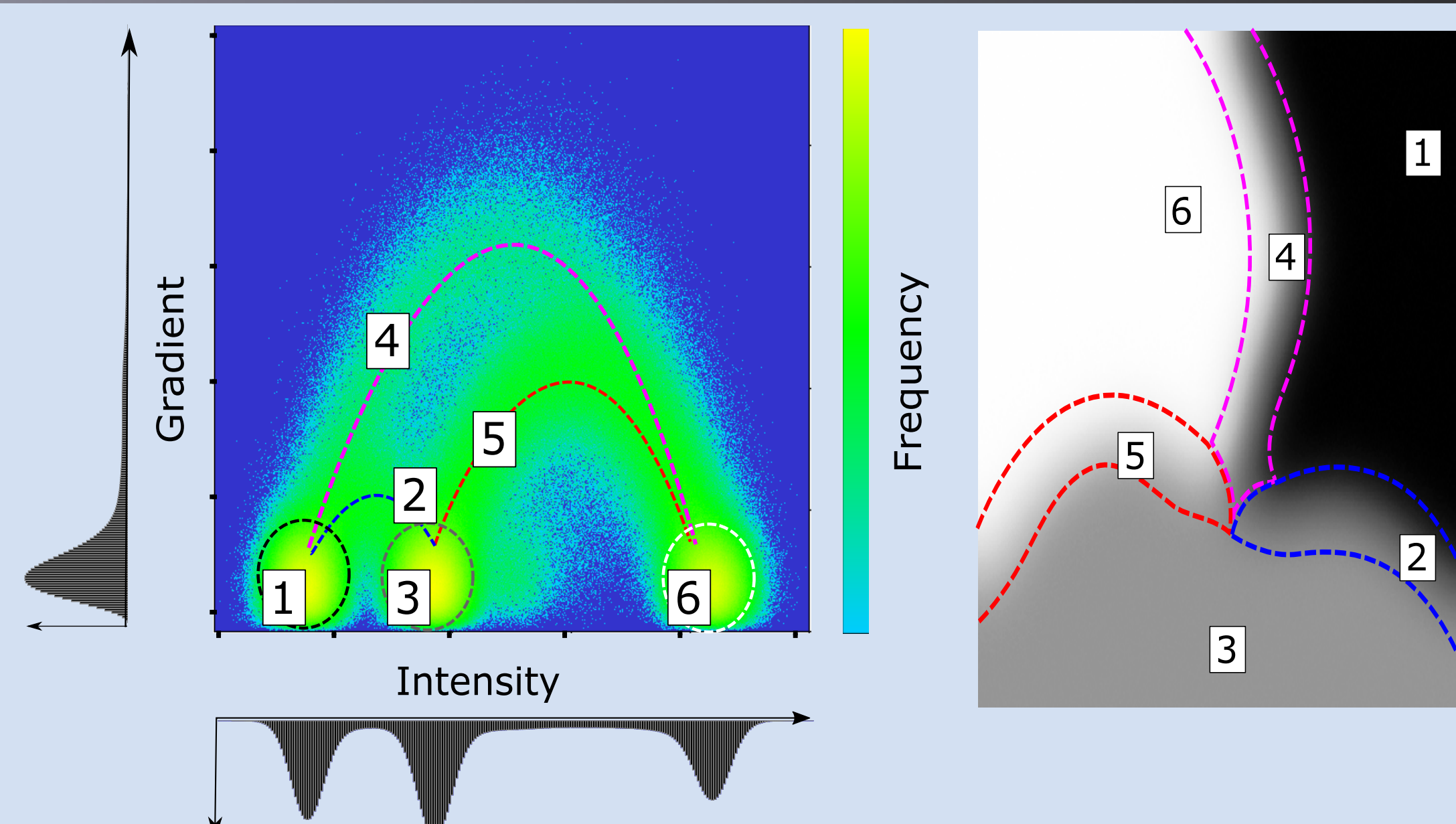
The ultimate goal of the project is to model the entire pipeline such that all sources of errors and uncertainty can be traced back to physical sources (e.g. material properties and data acquisitions parameters). This will in turn provide higher accuracy and enable assignment of meaningful error bars to the extracted material parameters.

References

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- 3 Jørgensen, P. S., et. al. Triple phase boundary specific pathway analysis for quantitative characterization of solid oxide cell electrode microstructure. J. Power Sources 279, (2015).
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An extended physical model

The first step towards extending the physical model is to look at the gradient in the image intensity data. The gradient of a pixel is a measure of how much its intensity differs from its neighbouring pixels intensities. Pixels in the phase interiors have a low gradient, while pixels on the interfaces have a higher gradient. Moreover, the resolution in the image data is related to the gradient magnitudes. By fitting a model to this data, we would expect to be able to extract interface areas and resolution in addition to the phase volume fractions and noise levels.



2D intensity-gradient histogram. The circles indicate the phase interiors while the three arcs correspond to the three types of interfaces in the material.

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