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Flexible 3D Tomographic Alignment and Reconstruction of Phase-Contrast Projection Data

<u>Tiago Ramos</u>^a, Jakob S. Jørgensen^b, Jens W. Andreasen^a

^a Technical University of Denmark – Department of Energy Conversion and Storage, Roskilde, Denmark ^b Technical University of Denmark – Department of Applied Mathematics and Computer Science, Lyngby, Denmark

Motivation: The performance of numerous engineering materials is determined by their internal structure right down to the micro and nano-scale. The use of high-resolution tomography allows an **accurate quantification of the microstructural parameters** of a testing sample and can provide useful information regarding its behaviour *in situ, in operando,* its degradation or failure mechanism, inter-phase connections, electrochemical properties, among others. The use of phase-contrast tomography (ptychography) has allowed tomography users to increase X-ray projection spatial resolution up to 8 – 10 nm, but 3D reconstructed models still can only achieve lower resolutions due to generated artefacts and positioning uncertainties during the measurements. We propose a fully automated alignment and reconstruction algorithm that avoids phase unwrapping operations, corrects linear background gradients in the projection data and is able to include all the angular and linear parameters that describe the scanning geometry.

The Alignment procedure:

We propose an automated alignment and reconstruction routine that takes into consideration the linear and angular parameters that describe any sample-detector relative orientation and is insensitive to phase wrapping and phase ramps.



The tomographic reconstruction algorithm:

We have extended the SIRT iterative algorithm to phase-contrast projection data, avoiding phase unwrapping operations that may generate artefacts in the reconstructed tomogram.





Reconstruction results before alignment: Tomographic reconstruction before projections alignment and wrapped phase sinogram.

Tomographic Reconstruction



Detected Air Region Ramp Corrected Projection



Detected Air Region



 $x^* = \operatorname{argmin} \left\| b^{\operatorname{PRR}} - \mathbf{A} \cdot x \right\|_{\operatorname{PR}}$

Fine Alignment Optimization $\boldsymbol{\Theta}^{\text{FPA}} = \operatorname{argmin}_{\boldsymbol{\Theta}} \frac{1}{2} \left\| \boldsymbol{b}^{\text{PRR}} - \boldsymbol{A}(\boldsymbol{\Theta}) \cdot \boldsymbol{x} \right\|_{2}^{2}$



Resolution gain quantification: Fourier Shell Correlation (FSC) measurements before and after the fine alignment procedure suggest a possible significant increase in the attained tomographic reconstruction resolution.

Conclusions and ongoing work: Final



Parallel beam experimental Setup: Undesired sample movements can be decomposed in a linear combination of the angular parameters α , β and θ and translation parameters **u** and **v**.

reconstruction resolution can be improved by means of the proposed optimization technique. The introduction of tilting parameters optimization can improve the sample reconstruction as demonstrated in the results. The proposed algorithm is currently being applied to real synchrotron data. Future work will be focused on the combination of phase retrieval methods along with the Fourier slice theorem in order to avoid projection translations corrections.

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