Toward *In Situ* Mapping of Crystal Selection during OFZ Crystal Growth

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Here, we present an automated and rapid method for nondestructive mapping of crystal grains in a rod-shaped sample. The approach was designed for application to in situ float-zone crystal growth experiments at an X-ray synchrotron source but could be useful in other applications. The methods have been tested on a TiO_2 boule grown in an optical float-zone furnace. The approach applies a statistical filter to polycrystalline diffraction patterns on two-dimensional (2D) detectors to rapidly determine the degree of powder quality of the signal. When larger crystals emerge in the growth, their position, size, and shape can be tracked using an automated blob-tracking algorithm that follows individual Bragg peaks as a function of position in a grid scan, even when multiple crystals are contributing spots to diffraction images. This method is found to be robust as the same crystal shape can be independently reconstructed using different sets of Bragg reflections. Image segmentation methods are then used to map out the polycrystalline grains. We also note that other information about crystal quality, such as mosaicity or strain state, may be inferred and mapped from the intensity variation of the Bragg peaks at different locations within the sample.

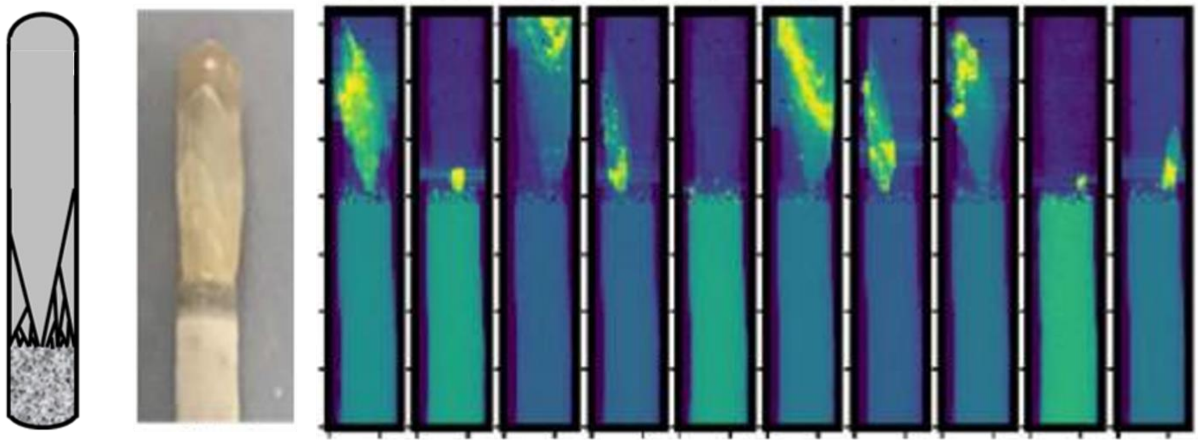

Figure 1: Schematic (left), photograph (center) and tracked grains (right) from a crystal growth boule that is the product of an optical floating zone (OFZ) crystal growth of TiO_2. The sample boule is about 5 mm in diameter with the crystal growth occurring over a ~20 mm length that is fused to the polycrystalline seed rod.

References

[1] - P.G. Khalifah, C.J. Wright, E. Dooryhee, L. Pressley, W.A. Phelan, and S.J.L. Billinge, Chem. Mater., *accepted*, (2021). https://doi.org/10.1021/acs.chemmater.1c00602