Tomographic Surface X-ray Diffraction

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Surface X-ray Diffraction (SXRD) is a powerful tool in surface studies due to its unique ability to determine atomic structures with great precision under working conditions. However, the method is currently limited to simple samples such as single crystals. We are aiming to develop Tomographic Surface X-ray Diffraction (TSXRD) as a tool for in-situ and operando surface structure determinations on polycrystalline samples. This will give new possibilities in the investigation of the relation between surface structure and function in many processes and devices, such as catalysis, electrochemistry, and corrosion.

Determination of grain orientation in the surface region can be performed similarly to 3D-XRD. There, Bragg reflections are used to extract spatially resolved grains of different crystalline orientations [1,2]. In TSXRD, similar tomographic approaches are used but with a focus on the Crystal Truncation Rods (CTRs) and superstructure rods to extract information about the surface structure and structural changes of each grain.

We have performed measurements of polycrystalline surfaces of different materials and grain sizes with clean and oxidized surfaces ex-situ. Presently, spatially resolved orientation maps of the surface region are being extracted. In parallel, we are developing the TSXRD analysis to extract the surface structure of both clean surfaces, surface reconstructions, and thicker oxide layers. We are currently able to distinguish some grains in the samples (see Fig. 1) and their crystalline orientation. In this presentation, we will describe the method in more detail and give an update on the analysis development.

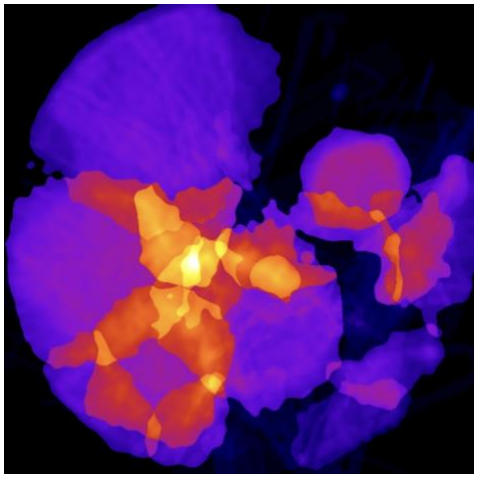

Fig. 1. Grains found in the near surface region of a polycrystalline palladium sample from measurements at P21.2 at PETRA III at DESY

[1] S. Schmidt, Journal of Applied Crystallography, **47**, 276-284 (2014)
[2] E. M. Lauridsen, Journal of Applied Crystallography, **34**, 744-750 (2001)