



Institute for Materials Science
Universität Stuttgart

**Colloquium
Materials Science
Summer Semester 2021**

On-line per WebEx !

Meeting number: 121 506 8121

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5th July 2021 @ 4:30 PM
**“3D Electron diffraction
(3DED) on oxides – solving
challenging crystal structures
from functional nano particles”**

Abstract: Many important materials, ranging from alloys, minerals or catalysts to framework compounds and pharmaceuticals are not suitable for growing large crystals prohibiting single crystal X-ray analysis. Yet, the introduction of nano crystallinity and special crystallographic features like disorder, defects, pseudo symmetry or stress/strain effects creates new or allows optimizing existing physical properties. With increasing complexity of the structures and special structural features as well as with decreasing size of crystalline domains, X-ray powder diffraction becomes difficult for structural characterization, fundamental for understanding material properties. High-resolution imaging techniques in the transmission electron microscope (HR-(S)TEM) allow visualizing structural features directly at the atomic scale but require high electron dose of several thousand e-/Å²s causing beam damage. In the last two decades electron crystallography experienced a boost through the development of electron diffraction tomography. After data acquisition and processing strategies were developed for automated diffraction tomography (ADT) a big range of 3DED methods has been set up following different data collection strategies. A major difference between the methods lies in the imaging and diffraction strategies carried out in TEM/SAED or STEM/NED mode, both already proved successful for structure solution and refinement using single nano crystals. Significant differences appear for example if the size of crystalline domains in the regime of some tens of nanometer, sometimes even strongly agglomerated or for material which is highly beam sensitive. In this case STEM imaging is more reliable and special tracking routines could be developed (FAST-ADT). The potential of the FAST-ADT method for crystal structure analysis for a variety of nano-crystalline oxides like battery materials, catalysts, glas ceramics, ultra hard materials including special crystallographic features like twinning, intergrowth of polytypes, the quantitative analysis of defects like stacking faults will be presented.

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