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Combined phase contrast imaging and diffraction at extreme conditions for determination of kinetic parameters

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Very recently, it became possible to combine propagation-based phase contrast-imaging (PCI) and X-ray diffraction at extreme conditions at the Extreme Conditions Beamline (P02.2), PETRA III, DESY, Hamburg. This first platform for such experiments enables the investigation of hierarchical structures at conditions approaching those observed in the internal structure of planets, with pressures exceeding 10,000 atm. In PCI, the incident X-ray wave front gets modified by the complex refractive index of the material and the propagation provides the phase information as measurable intensities. The partially coherent X-ray beam produces edge-enhancement in PCI, which provides strong contrast at phase boundaries revealing information on crystallization, solid-solid phase transitions and melting. Therefore, PCI can overcome the complications with absorption-based techniques, which are not useful for low-Z materials and for materials with small density differences. A successful flat-field correction is achieved by computing the principal component analysis (PCA) components on all images and finally to obtain the image in the object plane, phase retrieval algorithms are necessary.
This project concerns how the PCI can be used to extract information about kinetics of a sample system through the observation of micrometer-sized features, such as grain size. Meanwhile, X-ray diffraction is used as a secondary probe for sub-nanometer identification of the structural properties. The extreme states of matter are replicated using so-called diamond anvil cells (DAC) for pressure generation, which can be combined with infrared lasers to generate temperatures larger than 2,000 K. One further development of the DAC is the dynamic DAC, where, by applying a voltage profile to a piezo, the compression rate can be varied up to roughly 100 TPa/s. This enables the investigation of material properties –and kinetics –across a multitude of orders in magnitude in the compression rate.
Here, we are interested in simple systems, like gallium, pure water, and platinum, to test the capabilities of combined PCI with X-ray diffraction. We will describe our trials using standard segmentation analysis methods such as Chan-Vese segmentation, edge-detection and watershed, with that of the manual approach as well as a machine-learning approach and finally show that good agreement can be found between manually determining the size of grains and that found from segmentation using machine-learning. We will end with an outlook critically discussing the effectiveness of the machine-learning algorithms during data analysis and propose new ways of incorporating machine-learning into more parts of the project ultimately leading towards becoming a part of the beamline operation.

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