

Multi-modal Nanoscale Imaging of Materials and Biology

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A central challenge for imaging complex systems, such as metal defect structures or whole animals, is that information about features spanning multiple length scales is required. Furthermore, a complete understanding of the underlying properties can often only be achieved by correlating information from multiple techniques. Here we present a number of recent developments combining coherent diffractive imaging (CDI) at X-ray wavelengths with complimentary imaging and spectroscopy methods in transmission and Bragg geometry for rapid and high throughput imaging that provides multi-variable, 3D information about complex systems.

CDI is most commonly performed in the transmission geometry. This opens the door to simultaneously collecting multiple, complementary datasets, for example X-ray fluorescence or absorption spectroscopy data. For instance, a series of CDI measurements, spanning an adsorption edge, provides not only an image of the sample but contains chemical information in the form of XANES spectra at every image pixel, while fluorescence data allows for mapping of elemental distributions throughout the sample. The simultaneous data collection is paramount for dynamic systems such as the curing process of geo-polymer cement and *in-operando* electrochemical processes. Using ‘on-the-fly’ measurement approaches, where the sample is translated continuously, it is possible to image large areas that would have been prohibitively time-intensive using step scanning methods. The development of fly-scanned ptychography [1,2] enables the integration of CDI with existing instruments. An example of this is a recent study of metal distribution throughout the ultrastructure of *C. elegans* worms, measured at the XFM beamline of the Australian Synchrotron (Fig. 1). The 0.3 mm² area was collected as a single fly-scan in 180 minutes, consisting of approximately 5×10⁵ diffraction patterns with 47 nm wide effective sample pixels. Processed in parallel over 20 minutes, this represents a significant development, whereby biologically significant numbers of specimens can be investigated and their ultrastructure resolved to lengths smaller than the probe size.

The use of multiple measurements and combinatory experiments are also useful in crystalline materials subject to diffractive imaging in the Bragg geometry, called Bragg CDI (BCDI). BCDI provides both the crystal shape and spatially resolved lattice displacement information parallel to the scattering vector. By combining data from multiple, non-collinear reflections of the same crystal, the full strain tensor can be recovered. Aided by the development of robust alignment protocols [3,4], recovery of the stresses and strains is demonstrated for a highly strained gold crystal in the context of focused ion beam induced damage (Fig. 2). Here, ion induced damage effects are observed to modify the bulk material properties at length scales exceeding the ion penetration depth. This provides new fundamental insights

into the nature of damage and defect network structures across multiple length scales. Alongside this work, strain and X-ray induced damage within bio-crystals is discussed [5].

CDI employed on its own is a powerful imaging method. We have shown that when combined with spectroscopic or other additional information significant new insights may be brought to bear on a variety of complex systems. The continued development of rapid and high throughput CDI of both biological and materials science samples is shown to aid in the understanding of dynamically evolving systems. Looking to future light sources, these developments are essential in ensuring that full advantage can be taken of the high coherence which will become commonly available at instruments.

References:

- [1] Deng, J. *et al.* Opt. Express **23**, 495–501 (2015)
- [2] Jones, M. W. M. *et al.* J. Synchrotron Radiat. **23**, 1–7 (2016)
- [3] Hofmann, F. *et al.* J. Synchrotron Radiat. **24**, (2017)
- [4] Hofmann, F. *et al.* Sci. Rep. **7**, 45993 (2017)
- [5] Coughlan, H. D. *et al.* Struct. Dyn. **2**, 41704 (2015)

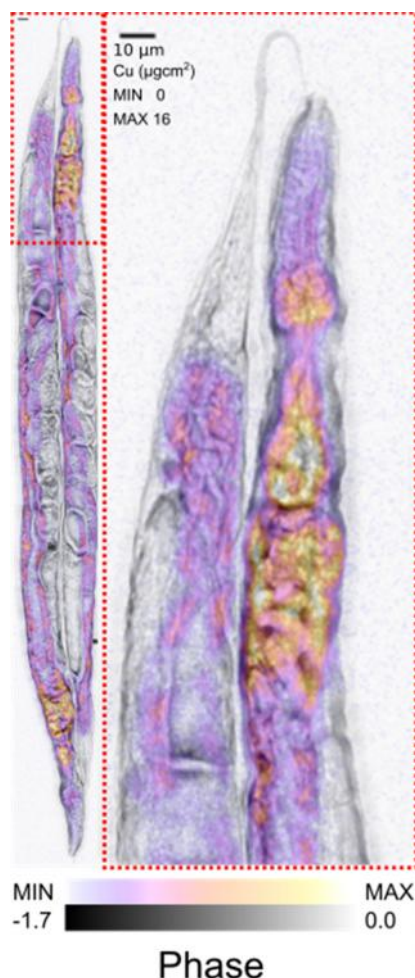


Fig. 1. The reconstructed phase of two *C. elegans*, overlaid with simultaneously collected Cu fluorescence. All scalebars correspond to 10 μm .

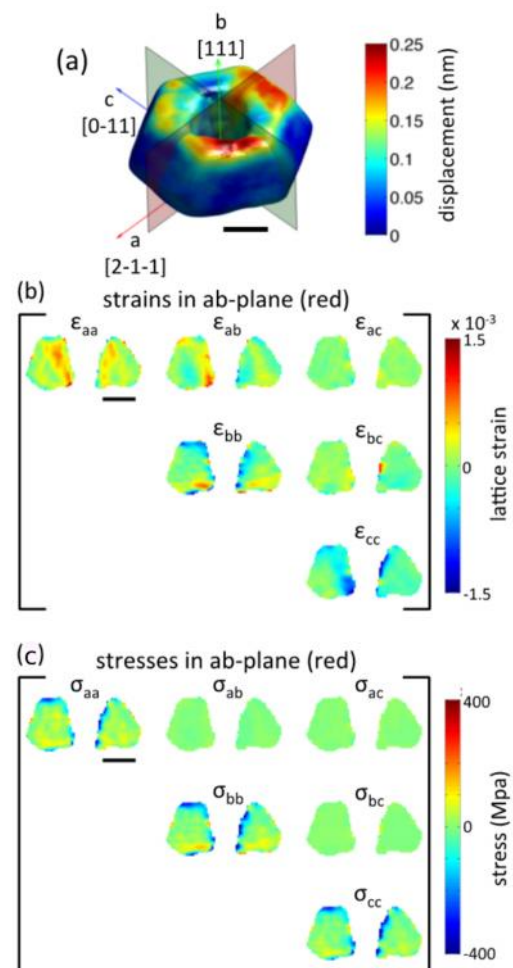


Fig. 2. Reconstructed strains and stresses in an Au micro-crystal with a hole milled through the center. A cross-section of the annulus-like shaped crystal is shown in b) and c). All scalebars correspond to 300 nm. Adapted from [3].