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Towards joint high-pressure X-ray and neutron single-crystal diffraction

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Diffraction methods can provide the highest-quality structural information about a crystal on the atomic scale and much work has been carried out to adapt X-ray and neutron diffraction techniques to a variety of challenging sample environments, including high-pressure. The ability to influence directly intermolecular distances makes high pressure one of the most important tools at our disposal for answering one of the big questions in chemistry - the prediction and control of solid-state structure.

Modern neutron Laue diffractometers with large image-plate detectors permit extensive continuous sampling of reciprocal space with high resolution in the two-dimensional projection and a wide dynamic range with negligible bleeding of intense diffraction spots, qualities that are highly suited to high-pressure crystallography [1].

Here we show that high-pressure single-crystal neutron diffraction data can be collected using Laue diffraction from a sample of hexamine in a miniature diamond-anvil cell (mini-DAC) with no significant reductions in completeness or resolution [2]. The data are of similar quality, as judged by R-factors, geometric parameters, and estimated standard deviations, to those obtained at ambient pressures. This is achieved by the ability to measure diffracted intensity directly through the body of the mini-DAC.

Joint high-pressure experiments using both X-ray and neutron diffraction on the same sample are now feasible using the mini-DAC and modern neutron Laue diffractometers like KOALA on the OPAL reactor.

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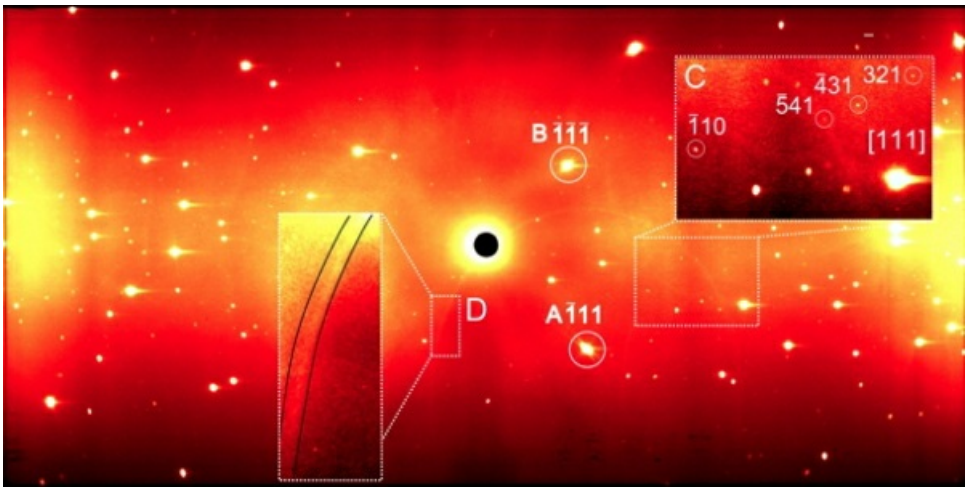
[2] Binns, J., Kamenev, K. V., McIntyre, G. J., Moggach, S. A. & Parsons, S. (2016). IUCrJ, 3, 168-179.



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