Wombat – the high intensity diffractometer at OPAL

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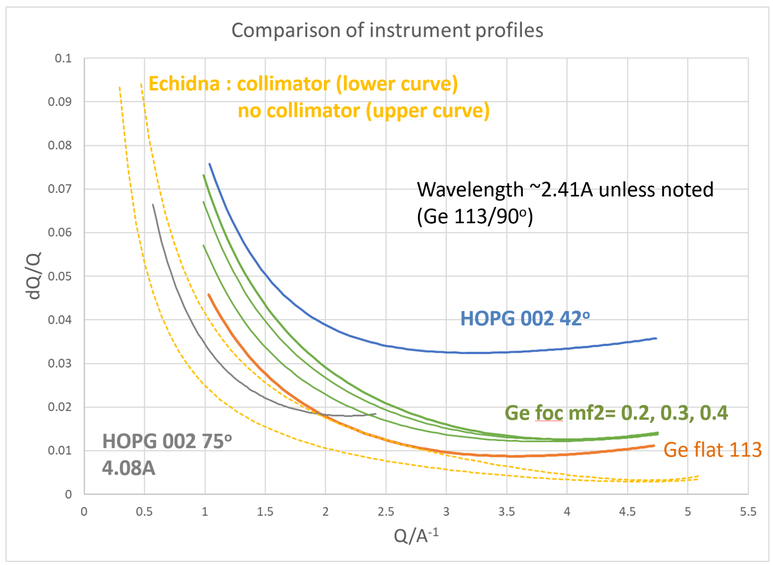
Wombat is more than merely fast: it operates over a broad configuration space of resolution and intensity.

Wombat- The Instrument

Wombat is the high intensity neutron diffractometer located in the OPAL Neutron Guide Hall. Its high resolution counterpart, Echidna is located downstream on the same guide. Wombat is an open geometry instrument (no collimators). It is primarily used as a high-speed powder diffractometer, but has also expanded into texture and single-crystal measurements.

Wombat combines a 120º x 15º area detector with excellent timestamping capabilities (for time resolution) with 300x50mm neutron guides and vertically focusing monochromators (for flux). An oscillating radial collimator rejects extraneous sample environment scattering.



Wombat: Configurability

Wombat has a continuous takeoff angle range 40º-120º. Three monochromators are available.

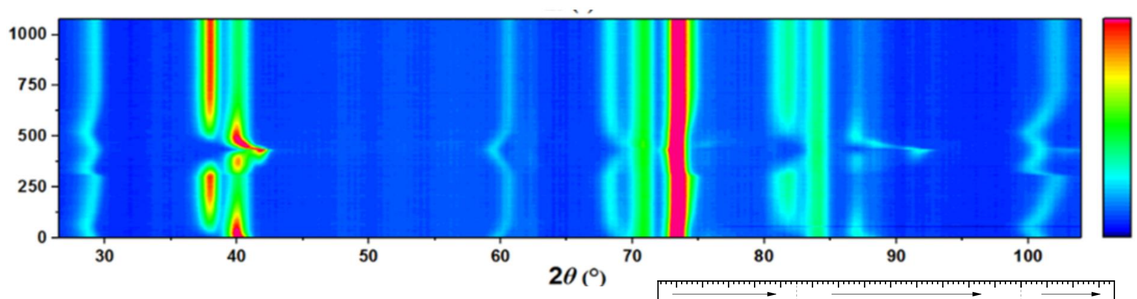
- High resolution flat Ge 335 (113, 115, 224 available; 1-3A)
- High intensity focusing Ge 115 (113, 335, 224 available; 1-3A)
- High intensity/ high wavelength HOPG 002. (2.4A, 4-6A)

HOPG and Cooled Be filters available.

A wide range of ancillaries: dilution to 50mK; cryo 1.5-300K, 4-800K; vacuum furnace 300K-2000K, environment furnace 300K-1300K. Neutron polarization and analysis. Magnetic field to 11T. High voltage to 20kV. High pressure to 10GPa. Many of these concurrently.

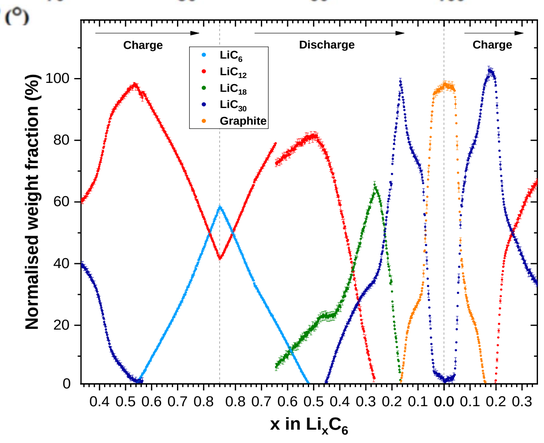
Rapid real-time structure for *in-operando* battery cycling

Wombat is capable of real-time one-shot measurements down to 20ms. In this case the standard Ge monochromator was used for *in-operando* battery cycling measurements with 10s time resolution (at time of publication the fastest reported battery measurement)



Above: Diffraction pattern vs run number (vertical), each run is 10s.

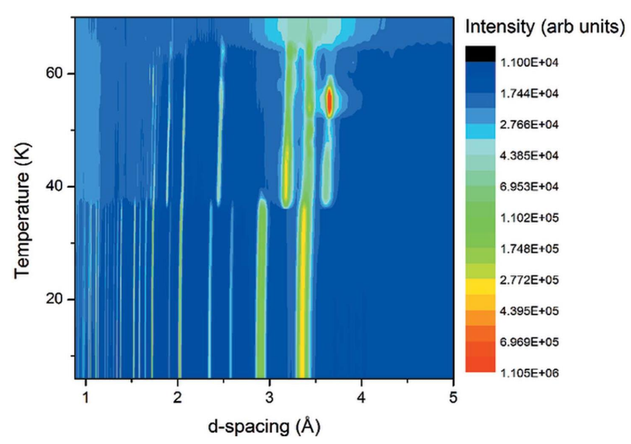
Right: derived weight fractions vs lithium loading over the charge cycle. Note that, even for fast measurements, high quality refined information can be extracted from the data. Note, for example, the LiC_{18} phase present only during delithiation

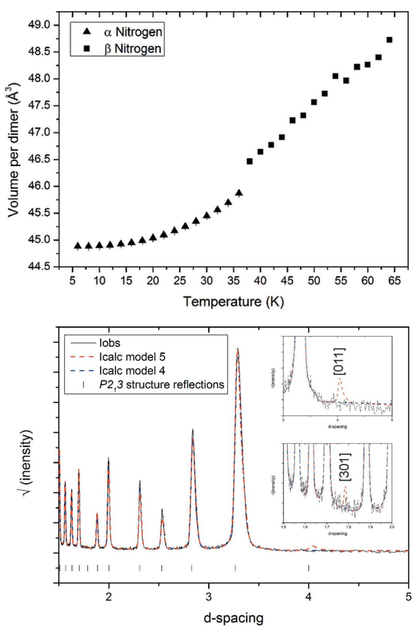


Liang, Didier, Guo, Pang & Peterson, *et al, Adv. Mater.* **31**, 882-886 (2019)

Parametric structure determination with exotic consequences

Wombat was configured in the higher resolution Ge 335 monochromator mode to determine phase and lattice parameter behaviour in (undeuterated!) CH_4 and N_2 in the 5-80K range. Despite their ubiquity, the solid phase temperature behaviour of these materials was not well understood. This has potential consequences for geological behaviour on outer- Solar System bodies such as Pluto.





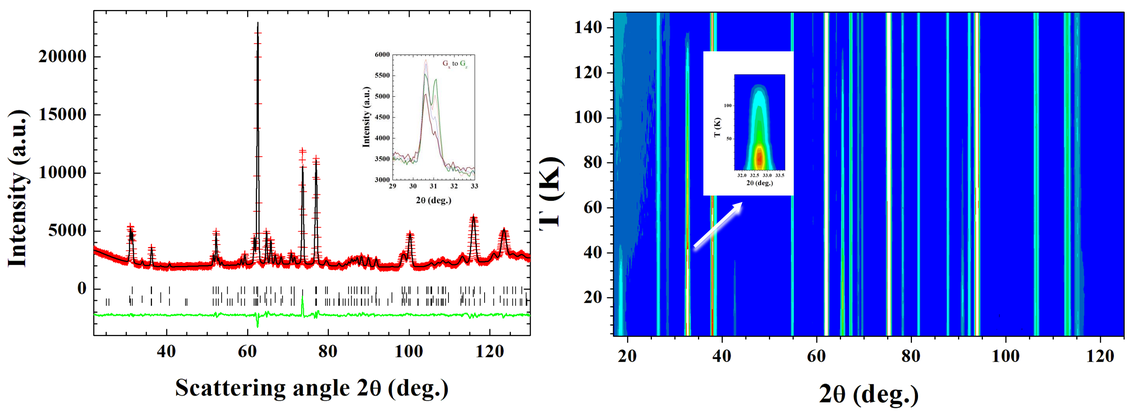
Above: Diffraction map vs temperature for N_2. Top right: high resolution mode yields accurate refined parameters. Bottom right: the appropriate balance of resolution with intensity allows model discrimination due to systematic absence to be conducted with confidence.

Maynard-Casey, Hester & Brand, *IUCrJ* **7** 844-851 (2020)

Magnetic structural determination in small samples

Wombat was configured with the higher resolution Ge 335 monochromator mode to investigate magnetic structural transitions in a 35mg sample synthesised under high pressure. In this case the resolution at low Q was sufficient to resolve the magnetic transition. (3hr per pattern)

Wombat was also used with the Ge 113 focusing monochromator to study low temperature ordering in a 90mg sample (15min per pattern). These two examples show that, even with weak scatterers, Wombat can be tuned to an appropriate resolution to suit the science.



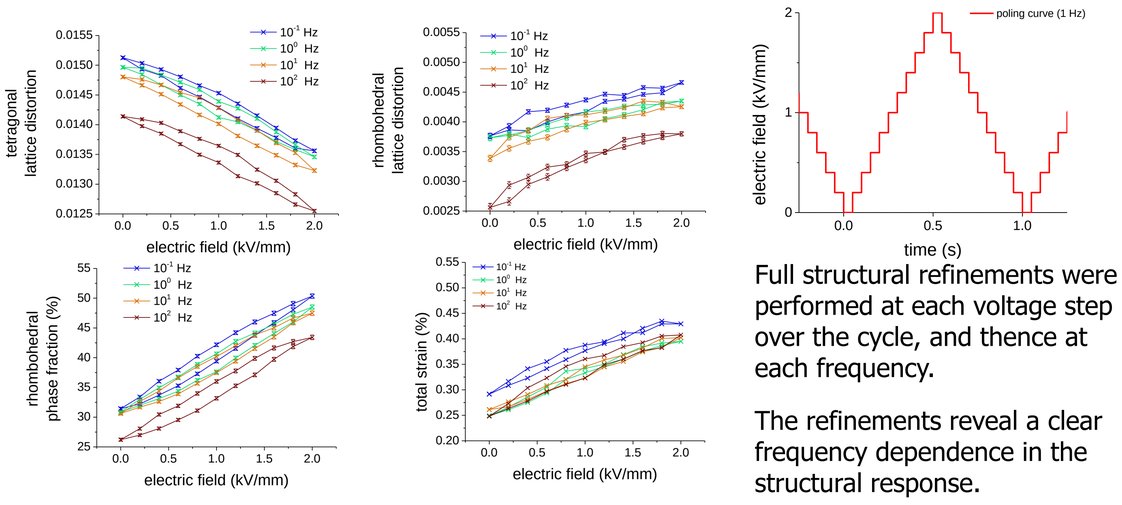
Left: dataset in high resolution mode, inset shows change in magnetic ordering with temperature. Right: diffraction map showing low temperature magnetic ordering. Both datasets collected at 2.41A.

(Chin-wei Wang *et al.,* in preparation)

Stroboscopic diffraction in piezoelectric materials

The detector can be synchronised to external sources such as pulse generators to perform high frequency cyclical measurements. Time resolutions down to 20ms are possible and 1kHz measurements with multiple time bins are routine *even in the higher resolution mode.*

In this example, a standard PIC151 sample was subjected to a trapezoidal voltage for several frequencies. The sample was measured at multiple rotations to resolve the textural effects induced by the field.



Full structural refinements were performed at each voltage step over the cycle, and thence at each frequency.

The refinements reveal a clear frequency dependence in the structural response.

Above: refined structural parameters in PIC151 over a cycle at several frequencies.

(Manuel Hinterstein *et al.*, in preparation)