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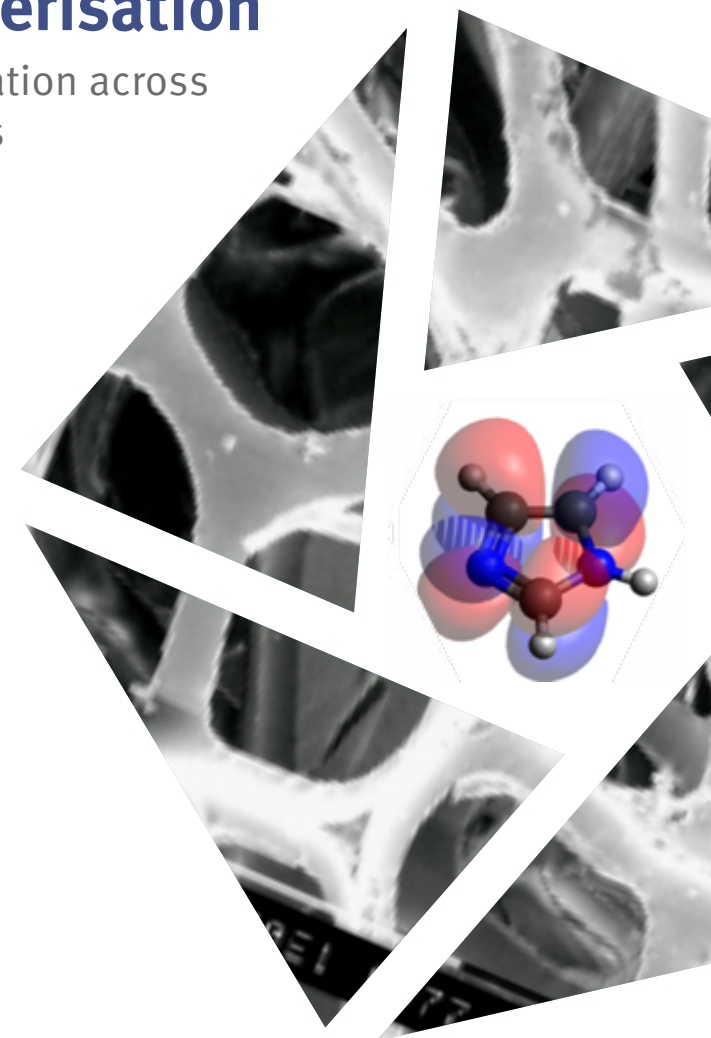
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CMAC
FUTURE MANUFACTURING
RESEARCH HUB

Advanced Measurements & Characterisation

Spatial organisation across
all length scales



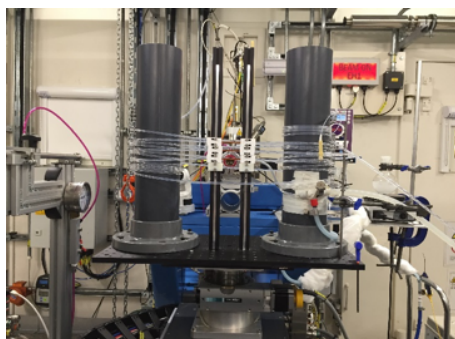
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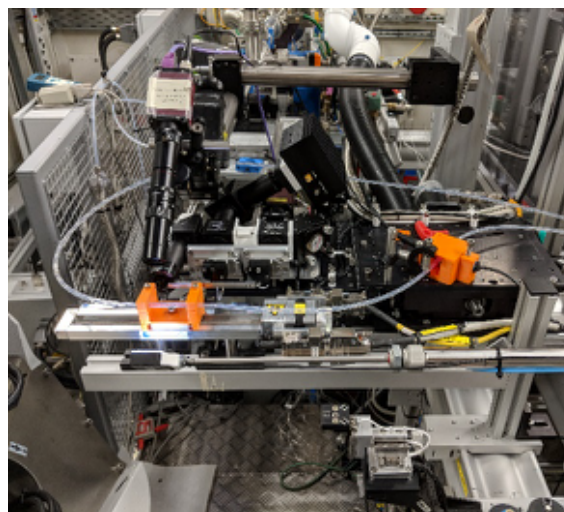
Through its research team on the UK Science and Innovation Campus at Harwell (Oxfordshire) CMAC works seamlessly with the UK's central facilities – the Diamond synchrotron, the ISIS neutron source and the Central Laser Facility. The group is based in the Research Complex at Harwell, which is available as a 'research hotel' for all CMAC partners, for long and short term projects leveraging the advanced measurement facilities at Harwell.

Using advanced characterisation techniques, we aim to develop molecular level understanding of the systems at various stages of the workflows and end-to-end process design."

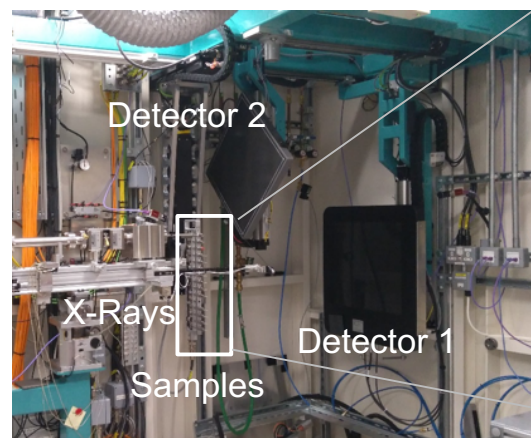


KRAIC-D set up in Beamline I11

CMAC researchers from the University of Bath have developed time-resolved diffraction methods to follow the crystallisation of APIs in a continuous flow process. For example, the bespoke KRAIC-D segmented flow reactor was installed on the powder diffraction Beamline I11, where it was used to follow the complex phase transformations during carbamazepine crystallisation in real time. On the single-crystal diffraction Beamline I19, a larger-scale segmented flow set-up has been commissioned, which enabled the first in situ collection of single-crystal diffraction images from paracetamol crystals grown in flow at millisecond time resolution.



KRAIC-S set up in Beamline I19

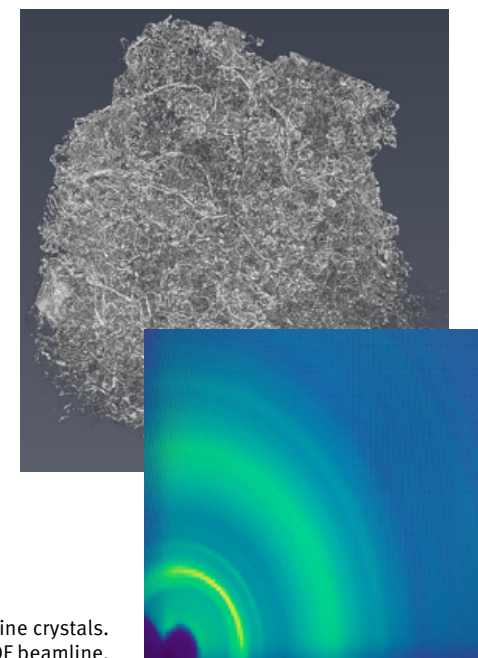


I15 Beamline set-up to automatically determine the PDF of solid samples.

CMAC researchers from the University of Strathclyde are using phase-contrast X-ray imaging with sub-micrometer space resolution and sub-second time resolution to control and visualise phase transformations in continuous twin-screw extrusion process for API-polymer formulations. Their studies are underpinned by time resolved pair distribution function (PDF) measurements that allow correlation between structure at the molecular scale with mesoscopic and macroscopic information from the imaging studies. Amorphous drug-polymer systems, were tracked in variable temperature experiments. The data allow a better understanding of the impact of process parameters on non-crystalline formulations.

CMAC researchers at the University of Leeds are carrying out in situ analysis of mixing, nucleation and crystal growth in continuous flow systems. For example, phase contrast X-ray tomography of glycine in an anti-solvent crystallisation process revealed the complex nature of the solid product, visualising the influence of the flow-field on product morphology.

Using in situ X-ray Raman scattering, X-ray photoelectron spectroscopy and time-dependent density functional theory it has been demonstrated that monitoring the 1s core level spectra of carbon, nitrogen and oxygen provides a powerful probe for monitoring local bond formation and breaking. This enables studies of nucleation from solution with unprecedented insight into molecular association processes in the metastable zone.



Top: 2D reconstruction of glycine crystals.
Bottom: Diffraction patterns at I15 XPDF beamline.