CMAC
FUTURE MANUFACTURING
RESEARCH HUB

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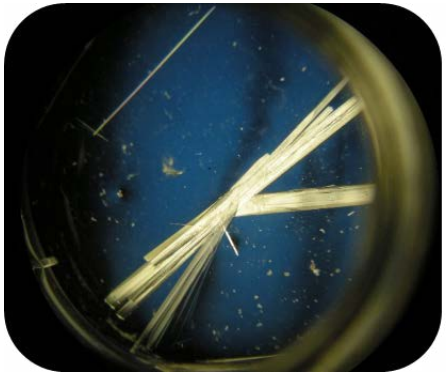
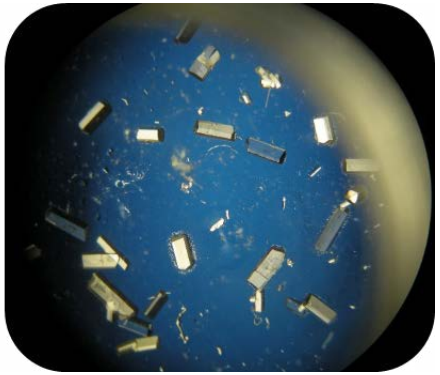
Additive & Morphology Control

Towards rapid assessment, prediction and integration

EPSRC
Engineering and Physical Sciences Research Council

Additive & Morphology Control



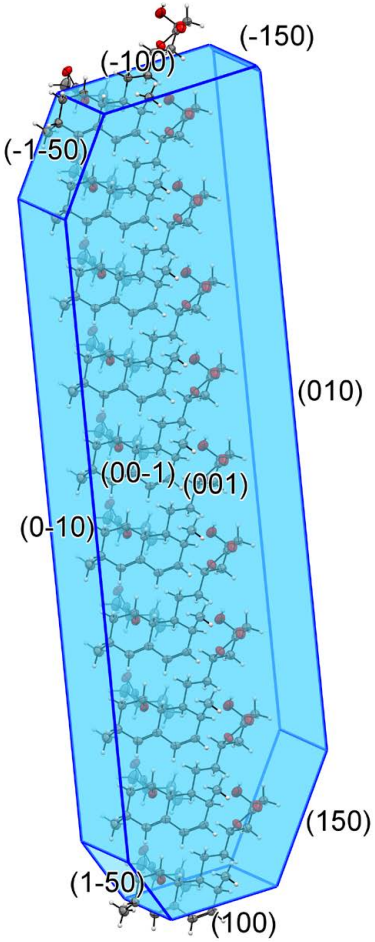


CMAC researchers across the Hub are undertaking research to develop a workflow that rapidly assesses the feasibility of using additive crystallisation to control the morphology of the particles formed and that is capable of being integrated into an end-to-end process to design a microfactory prototype.

Additives can be small molecules or polymers, that influence the crystallisation process but are not themselves incorporated in the final product. The Additive workflow will sit alongside the existing cooling crystallisation and antisolvent crystallisation workflows that have been developed by CMAC so we can quickly assess which method is most suitable for a particular Active Pharmaceutical Ingredient (API).

The additive crystallisation workflow development will focus on rapid assessment of ability to control morphology, improving reproducibility, and operating at a scale that can integrate with other unit operations within an end-to-end process. It builds on previous work in CMAC that demonstrated the first polymer additive control of morphology in a continuous crystallisation process.

Additives can be used to engineer crystal growth by adsorbing onto, and inhibiting growth on, selected crystal faces. This results in different shaped crystals being produced under different conditions and with different additives. Optimising crystallisation conditions in such a multi-component environment represents a significant challenge in both academia and industry.



The Additive & Morphology research programme includes applying understanding and design of molecular interactions available from academic structural research in the selection of additives. A face indexing workflow has been developed and is being used to help predict how crystals will grow based on experimental measurements.

The predictive modelling aspect of the Additives & Morphology workflow element of CMAC digital design will, in the short term, be focused on particle attribute based models. Computational approaches to intermolecular interactions at the molecular level will target predictive design of additive-mediated primary particle control. This particle attribute based modelling work is being carried out in collaboration with the ADDoPT project. Process parameter models for additive-mediated crystallisations are a longer term goal.