Contextualising high explosive shock sensitivity relative to internal defect structures.

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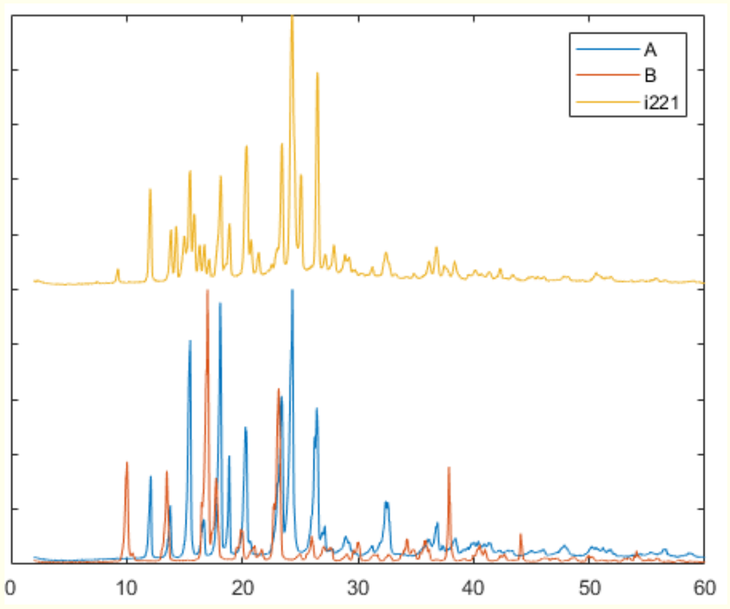
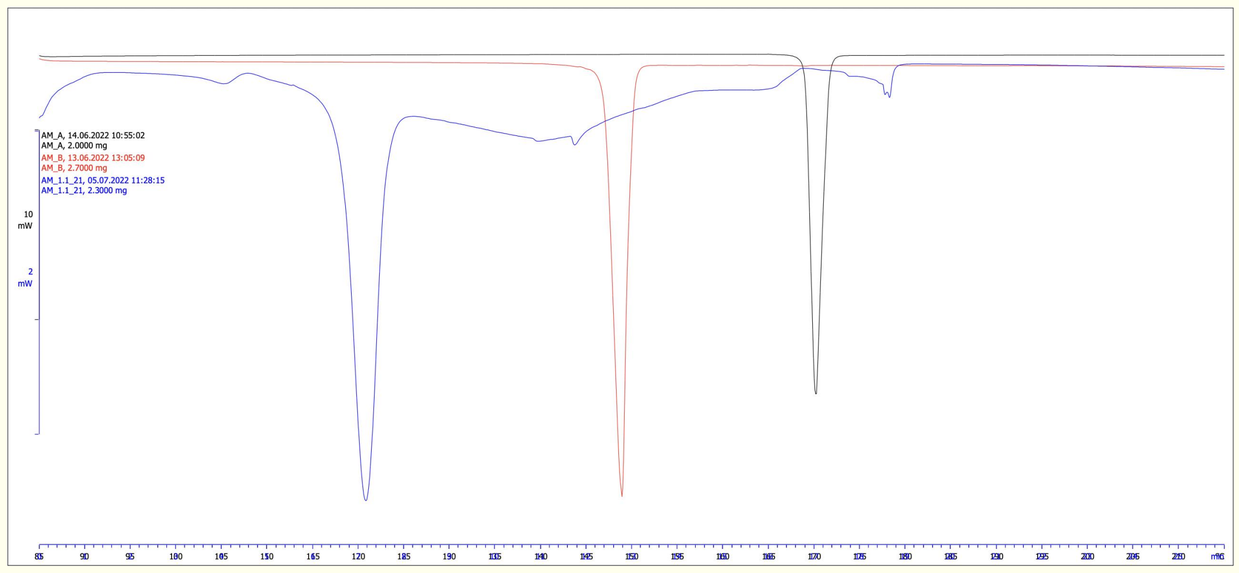
Introduction

Solid energetic materials are crystalline and contain structural defects. The build up of these in materials has significant effect on the stability of manufactured explosives.[1] Prior work has looked at RDX and PETN and it was noted that the microstructures changed depending on the method of recrystallisation and previous HMX studies found that this material exhibits crystal twinning.[2] It is known that paracetamol exhibits similar properties, which makes it a good inert analogue to do initial research on the topic[3], with known modifications of the basic structure. Initial studies of the paracetamol system are the basis for ongoing work with HMX.

Co-crystallisation

Graph 1





Graph 2

An array of paracetamol systems were grown from solution and show evidence of a complex array of co-crystals. Powder diffraction data was collected, showing the original materials of 4-acetaminophenol and 3-acetaminophenol (red and blue overlaid) and resulting system. The combination exhibits major differences in powder patterns, highlighting that co-crystallisation has occurred. This is supported by the DSC results. Collection of single crystals is now being undergone for single crystal structure determination studies.

Results

Single crystal paracetamol have successfully been produced, as shown in figure 1. The different faces have been identified and indexed which is shown in figure 2. The crystal shows a large volume of imperfections in the centre, close to the seed crystal, but greater levels of perfection can be seen as the crystal grows outwards from the centre.

Figure 1

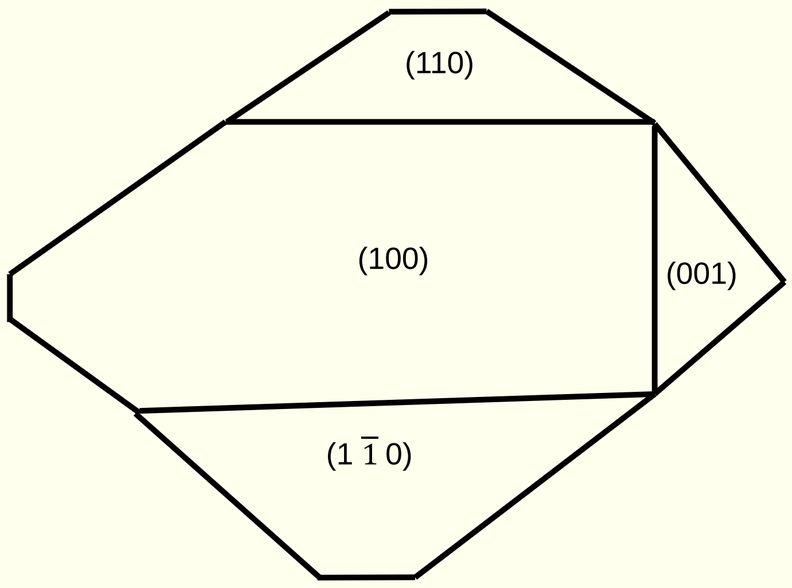


Figure 2

Future Work

Larger single crystal paracetamol will be grown before undergoing Xray topography to allow for the mapping of defects. The co-crystal work will be extended to examine RDX/HMX bb. Shock waves will then be passed through the crystals and the results correlated to the found defects. Altering the growth conditions will tune the defects present.

References

1. H. G. Gallagher, J. N. Sherwood and R. M. Vrcelj, *J. Cryst. Growth*, 2017, **475**, 192–201.
2. H. G. Gallagher, J. N. Sherwood and R. M. Vrcelj, *Chem. Cent. J.*, 2014, **8**, 75.
3. I. Andrusenko, V. Hamilton, E. Mugnaioli, A. Lanza, C. Hall, J. Potticary, S. R. Hall and M. Gemmi, *Angew. Chem. Int. Ed.*, 2019, **58**, 10919–10922