

MS41-P5 Advanced materials analysis with the powder diffraction file™

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Ten years ago the ICDD launched a new family of database products PDF-4. The purpose of these new databases were to provide researchers with an array of solid state analysis tools based on the powerful combination of single crystal and powder reference data, housed in a relational database format that could provide flexibility and powerful data mining. The ICDD has developed reference data and editorial procedures for experimental nanomaterials as well as amorphous materials. PDF-4 products now contain both amorphous and nanomaterial references. The use of digital patterns for both the material being analyzed and reference materials allows us to study crystallite size [1], molecular orientation and various instrumental and specimen contributions to the coherent and incoherent scatter, allowing for the analysis of crystallinity. Digital simulation tools are used to make the analyses radiation independent so that we can use experimental x-ray, neutron[2], electron [3] or synchrotron diffraction data for the analyses. We continue to work with our global membership to develop new methods and procedures. Most recently we have reviewed and published the largest collection of modulated structures, properly described by superspace groups, with up to 6-dimensional indexing and modulation vectors [4]. For improved quantitative analyses we have added massive numbers of atomic coordinates, digitized all patterns and calculated I/Ic scaling factors for both X-rays and neutron analyses.

References

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<http://www.icdd.com/products/2014/modulatedstructures.htm> and <https://www.youtube.com/user/TheICDD>

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MS41-P6 What pushes some molecular materials beyond the edge of crystallinity : an experimental study based on machine-learning predictive models

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Many molecular systems, perhaps a substantial minority, exist near the 'edge of crystallinity'. Often, despite repeated crystallisation attempts, these materials, at best, form polycrystalline solids and frequently exhibit substantial defects in crystal growth. Why is long-range order facile in some organic materials while others exhibit significant build-ups of defects and lattice strain?¹

We have recently established predictive models, developed using machine learning algorithms,² that provide a set of chemical and geometrical reasons why some materials crystallise more straightforwardly than others. Here, we present our initial experimental results from a set of 200 materials with unknown crystal structure that we predict using our machine learning algorithms to span the boundary between poorly crystallising materials and those which form single crystals.

Using the high resolution MAC detectors on ESRF beamline ID22, we have measured the powder diffraction patterns of all 200 structures. The materials are constituted into thirteen families, each containing a set of chemically similar derivatives. A substantial number of potential pharmaceutical materials are included in the study. While some structures are amorphous, most of the data are of sufficient quality to determine not only the crystal structure but also the extent and nature of microstructural imperfections such as lattice strain and stacking defects which are common and clearly visible.

Here, we will present an overview of the results, which includes analysis of *hkl*-dependent anisotropic and asymmetrical line broadening as well as particle-size distributions. With 200 organic materials, in thirteen chemical families, we have a substantial body of information that allows us to rationalise the difference in behaviour across families as functional group derivatives vary, and enables us to correlate the propensity for crystallisation with the degree of microstructural imperfection.

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