Structure determination of nanocrystalline organic compounds from unindexed powder data by real-space and PDF methods

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In my presentation I will show three methods for structure determination of nanocrystalline pharmaceutical compounds from uindexed powder data.

1. Fit with Deviating Lattice parameters (FIDEL) [1]

Classical real-space methods and Rietveld refinement require the lattice parameters to be known. If the lattice parameters are incorrect, the simulated peaks do not overlap with the experimental peaks. For this task, we developed a fit with deviating lattice parameters (FIDEL), which uses cross-correlation functions to compare simulated and experimental powder patterns. Starting from a large number of random structures with random lattice parameters in various space groups, the structures are fitted to the experimental powder pattern. The best matching structures are subsequently treated by Rietveld refinements. If the molecules are too flexible and/or the powder data are too bad, there can be multiple propsed crystal structures, which all fit to the experimental powder pattern sufficiently well.

2. Structure determination by fit to the PDF curve [2]

We are developing a similar procedure for structure determination, which performs a fit to the pair-distribution function instead of to the powder pattern itself.

3. Comparison of the PDF of an amorphous sample with the PDF of known polymorphs [3]

If polymorphic forms are known, the experimental PDF curve can be used to determine the local structure of pharmaceutical compounds, even if the compound is amorphous.

Application examples are shown for all methods.

References:

[1] S. Habermehl, P. Mörschel, P. Eisenbrandt, S. M. Hammer, M. U. Schmidt: "Structure determinations from powder data without prior indexing using a similarity measure based on cross-correlation functions", *Acta Cryst.* 2014, *B70*, 347-359.

[2] D. Prill, P. Juhás, S. J. L. Billinge, M. U. Schmidt: "Towards solution and refinement of organic crystal structures by fitting to the atomic pair distribution function", *Acta Cryst.* 2016, *A72*, 62-72.

[3] M.U. Schmidt et al., in preparation.