The elusive structure of nanocrystals

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Diffraction techniques have become the golden standard method for identifying and analysing mineral phases. Many scientist rely on the access to structural databases for phase identification and data processing via rietveld refinement and similar techniques. As most known minerals are identified and their structure are readily avialiable this is fairly straightforward. But what happens when you come across a mineral that has an unknown structure?

If crystals of >100 μm are avialiable, routine single crystals analysis can be preformed using the Shellx software [1] and data from a four circle diffractometer. However, many compounds do not form large single crystals. In these cases powder diffraction data can be collected and ab initio software such as superflip [2] can be used to solve the structure. But this requires that the space group or at the very least the unit cell can be indexed from the diffraction pattern. But when peak overlap is so severe that the space group and unit cell cannot be determined, the conventional crystallographic methods are powerless to solve the structure.

By measuring the pair distribution function and analysing it with the Liga algorithm developed by Pavol et al. [3] it is possible to determine the structure of nano-sized material from the PDF using the interatomic distances.

In this work we have found a new hydrated calcium carbonate, that had us confronted with all these challenges and we propose to solve the structure using the Liga algorithm and comparing the result with high resolution PXRD and HRTEM data. Future analysis will include Neutron PDF analysis to determine the structure of hydrogen in the sample.

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