POWDER DIFFRACTION & HUMAN KIDNEY STONES: SOS? A … SIZE OR STRAIN … (OR BOTH) EFFECT?

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It has long been declared (1997) **[1a,b]** and accepted since then that the GSAS-I software **[2]** was inappropriate to account for the X-ray powder diffraction patterns of Kidney Stones, and that more elaborate models than the ones offered with it were required. Such is not our experience from datasets collected at the High Resolution Powder Diffraction beamline CRISTAL in operation at the Paris SOLEIL synchrotron.

As demonstrated in the **figure 1** below, the key point while handling GSAS-I is to first use the available CW [constant wavelength] model profile 3 [PROF 3] to decide whether the largest contribution to the linewidth is due to a Size [the LX term] or Strain [the LY term] effect. In the latter case, one may then elect to use the CW model profile 4 [PROF 4] to improve the least-squares fit if need be by making use of the Stephens formalism **[3]**. Once the larger contribution has been least-squares refined, then the second one is in turn adjusted, yielding very decent FOMs (Figures of Merit) and R-factors. In some tricky cases, the only appreciable contribution comes from the LY term and no quantitative estimate of the size of the crystallites can be derived from the X-ray powder diffraction patterns.

In the case of Human Kidney Stones [KS], the end game is to try to measure crystallite sizes as reliably as feasible to relate them to Electron Microscopy measurements and eventually correlate them with Urinary or Nephrologic infection. This requires removing the microstrain [LY] contribution to the observed linewidths. The chemical composition of the KS yields a preliminary hint: Ca-oxalates **[CaC_2O_4,xH_2O]** suggest hypercalciuria (2<x<2.5) or hyperoxaluria (x=1) whereas Whitlockite **[$Ca_{18}Mg_2(HPO_4)2(PO_4)_{12}$]** if abundant enough may indicate a Urinary Tract infection **[4a,b]**. One example of each (namely, whewellite[x=1] and whitlockite) will be discussed in some detail.

Literature:

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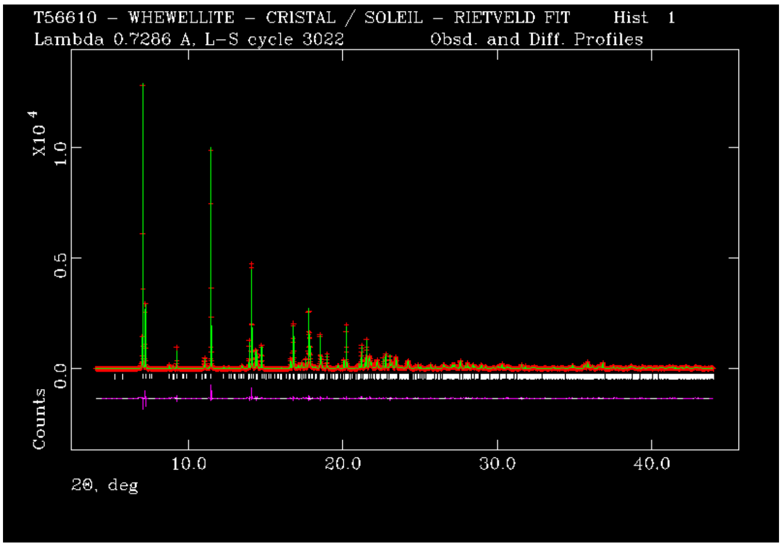

Figure 1: GSAS-I Rietveld refinement of a Ca-Oxalate monohydrate Kidney Stone: Whewellite [$CaC_2O_4.H_2O$]