Quantitative phase analysis in complex (and not so complex) mineralogical systems

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Quantitative phase* analysis (QPA) has its roots in the beginning of powder diffraction itself. While Debye and Scherrer were inventing powder diffraction [1-2], Hull [3-4] and Navias [5] were reporting QPA on various systems. After this, the use of diffraction for QPA was very much overtaken by those solving crystal structures, and it did not come back until the time of Alexander and Klug [6].

Powder diffraction, and by extension, QPA, is used extensively in many industries, such as minerals, pharmaceuticals, and cement, as well as in research in chemical engineering, chemistry, geology, physics, and materials science. The main thrust behind the desire to use diffraction to find out how much of each phase is present, is that the diffraction signal is produced directly by the phase itself, and not inferred by some other measurement.

The mathematical basis of QPA is well understood and its application should be straightforward [7], but the application of the theory quickly runs into reality. The influence of instrument, specimen, and analyst has been studied in many round-robins, looking at the analysis of materials such as Portland cement [8], clays [9], iron ore [10], and pharmaceuticals [11], as well as the previous general QPA round-robin [12-13]. In general, they have found that common issues arise around specimen preparation, data collection, and analyst errors, and state that, amongst other things, ongoing education is key to mitigating these effects.

To this end, several examples of the application of QPA to mineralogical systems will be discussed and methods of results validation will be introduced. Limitations on QPA will be reviewed, and some general “recipes” for QPA will be given.

* “Phase” means a discrete material with a common structure, which may or may not be crystalline. It has nothing to do with “phase” in the sense of the phase problem in X-ray crystallography.