

RIETVELD QUANTITATIVE PHASE ANALYSIS OF MINERALOGICAL MATERIALS

Mati Raudsepp

Department of Earth & Ocean Sciences, The University of British Columbia, Vancouver, BC V6T 1Z4, Canada

Advances in basic and applied research in the earth sciences depend significantly on knowing the identities and relative abundances of the constituent minerals of earth materials. Among the many experimental techniques now available for this purpose, X-ray powder diffraction stands out as one of the most powerful, yet still relatively simple to do. From an X-ray powder diffraction pattern, diffractionists may solve and refine the crystal structures of new minerals, identify minerals by matching to various standards databases, assess crystallite size and strain in very fine grained materials, and the most relevant here, measure the relative amounts of minerals in earth materials, whether they be sediments, rocks, products of mineral processing, or mine wastes.

Traditional methods of quantitative phase analysis (QPA) are many. Some examples are point-counting of thin sections or slabs of rock using an optical microscope, image analysis by scanning electron microscope or electron microprobe, and various conventional X-ray powder-diffraction measurements which make use of either single-peak or whole pattern methods. Mass-balance calculations (normative analysis) may also be used by which bulk chemical analyses are converted into mineral abundances of a prescribed set of minerals. While each of the traditional techniques of QPA may have merit in certain applications, none is as globally applicable and versatile as QPA using the Rietveld method with X-ray powder-diffraction data, which can overcome most limitations of traditional methods. Nevertheless, numerous pitfalls intrinsic to collecting any X-ray powder diffraction data such as specimen preparation, preferred orientation, microabsorption, and optimal refinement strategy must be overcome or, at least minimized, to achieve the best possible accuracy and precision of the measurements.

The mineralogy of mine waste and tailings determines the physical and geochemical stability of geological materials under different weathering conditions, and thus the nature and concentration of toxic, acid generating, or acid neutralizing chemical species that may be released. As the X-ray diffraction patterns of rocks and mine wastes are extraordinarily complex, with hundreds or even thousands of overlapping peaks, QPA of such materials is challenging. Here are given examples of the utility of QPA using the Rietveld method for the measurement of potentially acid-neutralizing carbonates in sulfide-bearing mine tailings, and coping with tailings containing structurally disordered phases, e.g., chrysotile and antigorite in kimberlite mine tailings.