EVALUATION OF POWDER XRD DATA USING THE MUDMASTER AND ROCKJOCK COMPUTER PROGRAMS

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Powder X-ray diffraction (XRD) analysis is a fundamental mineralogical method. In addition to qualitative identification of mineral phases, XRD is able to provide other important data. The presented contribution will focus on crystallite size distribution determinations and on quantitative analyses.

Size distributions for crystallites can be measured by XRD because the widths of the XRD peaks broaden as crystallite size decreases. The MudMaster program, written by EBERL *et al.* (1996), calculates crystallite thickness distributions (CTD) according to the Bertaut-Warren-Averbach theory (DRITS *et al.,* 1998). The BWA technique has been applied to measure CTD of kaolin minerals (ŠUCHA *et al,* 1999), to explore crystal growth mechanisms for illite and smectite (ŚRODOŃ *et al*., 2000; MYSTKOWSKI *et al*., 2000), to study diagenetic evolution of crystallite thickness distributions of illitic material (KOTARBA & ŚRODOŃ, 2000), to study weathering processes that affected smectite and illite/smectite (ŠUCHA *et al*., 2001), to measure fundamental illite particle thicknesses and to study crystallite-size changes of pyrophyllite during grinding, among other applications. From MudMaster analyses one is able to distinguish various geological processes. For example, thickness distributions of smectites show clear differences between primary bentonites and secondary, redeposited bentonites, because transport of primary bentonites decreases the mean thickness of smectite crystals. Weathering intensity is also revealed by measurement of kaolinite thickness distributions. Long and intense weathering produces thicker kaolinite crystallites than does less intensive weathering.

Accurate quantitative mineral analysis is important in many scientific and applied studies. ŚRODOŃ *et al*. (2001) described reproducible and accurate calculation of the mineral contents of rock by XRD when using an internal standard. EBERL (2003) wrote the RockJock program based on this previous work. The program fits the sum of stored XRD patterns of standard, pure minerals (the calculated pattern) to the measured pattern by varying the fraction of each standard pattern, by using the Solver function in Microsoft Excel to minimize the degree of fit parameter between the calculated and measured pattern. One of the advantages of the program is that it contains more than 90 standards that can be used with XRD data from most diffractometers. The list of standards contains common and less common minerals as well representatives of organic and volcanic matter. The program was used to determine of the quantitative mineralogical composition of clastic sedimentary rocks, bentonites, and alginates with good results.

Both programs, MudMaster and RockJock, are relatively easy to use. The latest versions of this software can be obtained by anonymous ftp from the Internet address: ftp://brrcrftp.cr.usgs.gov/pub/ddeberl/.

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