Rediscovering X-ray Diffraction in the Undergraduate Curriculum

John B. Brady and Robert M. Newton
Department of Geology, Smith College
Northampton, Massachusetts

Modern, computer-controlled powder diffractometers have made x-ray diffraction truly accessible to undergraduate students. Rugged, highly accurate goniometers that rarely need alignment, software-directed data acquisition and analysis, and on-screen comparison of data with powder diffraction standards leave sample preparation as almost the only non-keyboard skill required. These advances make it possible for students to concentrate on the information that can be gained from the diffraction experiment, rather than on the mechanics of data collection. Examples of student projects involving x-ray diffraction that have been completed by mineralogy students at Smith College include the following: (1) measurement of the lattice constants of several oxides with the periclase structure (MgO, CaO, MnO, NiO, SrO) to determine the relative sizes of the cations; (2) fitting of unit cells to powder diffraction data for minerals collected on field trips and comparing those data to the chemistry and unit cell parameters of similar minerals in the literature; (3) monitoring the progress of mineral transformations caused by heating including dehydration of portlandite to lime, crystallization of cristobalite from silicic acid, disordering of alkali feldspars, and homogenization of cryptoperthite; (4) identification of the fine-grained minerals in volcanic and low grade metamorphic rocks; (5) identification of the mineralogic constituents of very fine-grained materials such as soils, varved clays, and glacial till. Clay identification procedures involve mineral-transforming experiments such as expanding the clay layers by absorption of ethylene glycol and dehydration by heating. These projects, made possible by the acquisition of an NSF-ILI funded diffractometer, help move mineralogy courses beyond description and into the realm of experimental science.