Fourier Transform Analysis: (1) X-ray Diffraction Effects by Finite Montmorillonite and Mica Crystals

Malcolm Ross

U.S. Geological Survey, Washington, D.C. 20242

Abstract: A computer program has been developed to generate the X-ray diffraction intensity distribution along any particular reciprocal lattice row, plane, or volume, for any arbitrary group of atoms within a crystal. The program, which maps the intensity in crystal reciprocal space in much the same way as a conventional Fourier series program maps the electron density in direct crystal space, has been used to calculate the expected X-ray diffraction line profiles for a number of montmorillonite and mica crystallites of varying thicknesses in the *c** direction.

The program evaluates the function G(HKL)= $\sum$ n−1 N f n 2ni(H x n +K y n +L z n), where *G*(*HKL*) is the Fourier transform of an array of *N*-atoms at a particular *H, K, L* coordinate in reciprocal space, f_n is the scattering factor of the *n*th atom, and *x, y, z* its coordinates in direct space. The function is evaluated for all *N*-atoms within the finite model crystal under study for non-integral as well as integral values of *H, K,* and *L*. In practice a complete line profile is made by calculating *G* (*HKL*) at intervals in the range of (100 Å)$^{-1}$ to (10,000 Å)$^{-1}$.

The apparent *d*-spacings of the various clay mineral models, as given by the line profiles, approach asymptotically the true value as the number of layers increase. For example, the apparent d_{001} spacing for a mica of the composition K (Fe, Mg) 3 Si 3 Al 10 (OH) 2 is 12.91, 11.35, 10.79, 10.53, 10.38, 10.22, 10.14, 10.04 and 10.02 Å for crystals 2, 3, 4, 5, 6, 8, 10, 20, and 30 layers thick, respectively. For the infinitely thick crystal, d_{001}=10.000 Å. The apparent d_{001} spacing for a montmorillonite of the composition $K_{0.33}Al_2(Si, Al)_4O_{10}(OH)_2 \cdot 4H_2O$ (true d_{001}=15.400 Å) is 18.85, 16.80, 15.87, 15.52, and 15.41 Å for crystals 2, 3, 5, 10, and 30 layers thick, respectively.

These diffraction profiles and line shifts can be used in analyzing montmorillonites, micas, and mixed-layer montmorillonite-mica clays.

Clays and Clay Minerals; 1967 v. 15; no. 1; p. 47; DOI: 10.1346/CCMN.1967.0150105

Clay Minerals Society (www.clays.org)