FOURIER TRANSFORM ANALYSIS: (1) X-RAY DIFFRACTION EFFECTS BY FINITE MONTMORILLONITE AND MICA CRYSTALS

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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

$$G(HKL) = \sum_{n=1}^{N} f_n \exp 2\pi i(Hx_n + Ky_n + Lz_n),$$

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 nth 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 $(100\,\text{Å})^{-1}$ to $(10{,}000\,\text{Å})^{-1}$.

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

$$K(Fe, Mg)_3Si_3AlO_{10}(OH)_2$$

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.