Application of One-Dimensional Lattice Model to Mixed-Layer Muscovite-Montmorillonite

E-an Zen

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

Abstract: The one-dimensional Ising (regular solution) model is a first-order statistical mechanical approximation to real muscovite-montmorillonite mixed layer clays. The model assumes a constant excess interaction energy, w, between the unlike layers; w= w ab − 1 2 (w aa + w bb). Exact solution of the model, applicable to infinitely long chains, can be given by the quasi-chemical formula N aa ¯ N bb ¯ / N bb ¯ 2 =(1 4) exp (2w/kT) where N_{ab} is the equilibrium value of the number of $a-b$ type of neighbors, etc. When $w \rightarrow +\infty$, discrete crystals result; when $w \rightarrow -\infty$ and $N_a = N_b$, regular l:l mixed layer crystals result; when $w = 0$, random mixed layering results. For finite values of w, the mixed layering is irregular though non-random. Practically, however, either discrete or regularly mixed-layer crystals can obtain even for finite values of w calorimetrically too small to measure.

Using the Ising model, the values of w/kT and μ_i/kT (where μ_i is the excess chemical potential of the ith type of layers) were calculated for three clays whose probability of layer succession, p_{ij}, had been evaluated by the MacEwan method. For two muscovite-montmorillonite mixed layer clays, $w<0$; for a trioctahedral-dioctahedral mixed layer clay, $w>0$, as is expectable from crystallochemical considerations.

For thin plates of equal numbers of a, b layers, a correction factor $[(N-2)/N]^2$ (where $N = N_a + N_b$) must be applied even for ideal crystals. For such finite crystals, the partition function for non-ideal mixtures of specified N_a and N_b can be evaluated directly, introducing a second correction to the quasi-chemical relation. Because of end effects, it is possible that $N_{aa} \neq N_{bb}$ even for $N_a = N_b$ and $w = 0$, provided $w_{aa} \neq w_{bb}$.

Application of the Ising model to real crystals depends on our ability to correlate X-ray diffraction patterns with run sequences in crystals. Computer calculations of expected diffraction patterns for thin crystals having various values of N_a and N_b are being undertaken and should be useful towards this end.

Clays and Clay Minerals; 1967 v. 15; no. 1; p. 49; DOI: 10.1346/CCMN.1967.0150106