APPLICATION OF ONE-DIMENSIONAL LATTICE MODEL TO MIXED-LAYER MUSCOVITE–MONTMORILLONITE

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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;

$$w = w_{ab} - \tfrac{1}{2}(w_{aa} + w_{bb}).$$

Exact solution of the model, applicable to infinitely long chains, can be given by the quasi-chemical formula

$$\overline{N_{aa}}\,\overline{N_{bb}}/\overline{N_{ab}}^2 = (\tfrac{1}{4}) \exp(2w/kT)$$

where N_{ab} is the equilibrium value of the number of a–b type of neighbors, etc. When $w \to +\infty$, discrete crystals result; when $w \to -\infty$ and $N_a = N_b$, regular 1:1 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.