Nature of Structural Disorder in Natural Kaolinites: A New Model Based on Computer Simulation of Powder Diffraction Data and Electrostatic Energy Calculation

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Abstract: A new model for the description of the structural disorder in natural kaolinite materials is proposed, based on the stacking of two 1:1 layers and their enantiomorphs, and encompassing previously proposed models. The layers, where randomly stacked along the c axis (using probabilistic functions nested in recursive algorithms), correctly describe the observed powder diffraction patterns of natural kaolinites with any density of structural faults. The proposed model was evaluated using electrostatic energy calculations against earlier models of disorder based on layer shift, layer rotation, statistical occupancy of the Al octahedra, or enantiomorphic layers. The present 4-layer model has a minimum of potential energy with respect to the previous models. As expected, the fully ordered triclinic structure of kaolinite possesses the absolute minimum of potential energy.

Key Words: Energy calculation • Kaolinite • Layer disorder • XRPD simulation

Clays and Clay Minerals; August 1995 v. 43; no. 4; p. 438-445; DOI: 10.1346/CCMN.1995.0430407

Clay Minerals Society (www.clays.org)