High-Resolution Transmission Electron Microscopy of Mixed-Layer Illite/Smectite: Computer Simulations

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Abstract: High-resolution transmission electron microscope images of dioctahedral mixed-layer clay structures (illite/smectite) having various substitutional and polytypic schemes were modeled using computer simulation methods. Both one- and two-dimensional calculations were performed using parameters characteristic of a typical range of imaging conditions. One-dimensional images formed by imaging only 00/ diffractions show three important results: (1) The 20-Å periodicity resulting from rigorously ordered R1 illite/smectite can be imaged, but unconventional focus conditions may be necessary. (2) For crystals oriented with the electron beam perfectly parallel to the layers, the brightest fringes in the image correspond to either the octahedral sheets or the interlayer sites, depending on focus conditions. Misorientation of the crystal, however, by only 1° or 2° shifts the positions of the fringes by 1 to 3 Å. Furthermore, in tilted specimens, some defocus values produce images suggesting that smectite layers have a 11–13-Å periodicity, despite the uniform 10-Å periodicity present in the model structure. Thus, direct correlations between image and structure generally should not be made. (3) Two-layer polytypes of pure illite or pure smectite can also produce images with a 20-Å periodicity.

Two-dimensional images additionally showed that the cross fringes produced by some *hkl* diffractions can be imaged. The simulations showed that these cross fringes ideally might permit the determination of both layer stacking and compositional periodicity, but the fringes are lost by misorientations of a few degrees. These image simulations demonstrated, therefore, that mixed layering of illite and smectite theoretically can be directly imaged by transmission electron microscopy of chemically untreated specimens, but ambiguities may exist in the detailed intepretation of the images.

Key Words: High-resolution transmission electron microscopy • Illite • Image simulation • Mixed layer • Smectite

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