Variability in sepiolite: Diffraction studies

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ABSTRACT

Twenty sepiolites of known composition from different origins were analyzed to quantify the variability in structural parameters and its possible relationships with composition and morphology. Morphology SEM analyses led to classify the sepiolites into several groups, beyond the two simple macroscopic or clay groups. X-ray powder diffraction with synchrotron light was used to discuss the variability of the *a* and *b* cell parameters with the nature of the cations and occupancy of the octahedral shell. Rietveld refinement using the ideal sepiolite model is performed on sepiolites at two temperatures: 225 °C (for zeolitically dehydrated sepiolite) and 25 °C (for hydrated ambient sepiolite). The latter permitted to locate ca. six molecules of the zeolitic H₂O within the tunnels.

A few samples were selected to evaluate the feasibility and potential of single-crystal diffraction methods: X-ray microdiffraction and electron diffraction. The macroscopic sepiolites gave well-structured and rich X-ray fiber diffraction patterns, in excellent agreement with ab initio simulations. High-quality single-crystal electron diffraction patterns for three axis zones are indexed and compared with simulations. The experimental and modeling results for X-ray microdiffraction and electron diffraction open a new path for quantitative crystallography on sepiolite and other fibrous clays from the sepiolite-palygorskite group.

Keywords: Sepiolite, X-ray diffraction, Rietveld, 2D diffraction pattern, SEM, TEM, SAED, ab initio simulations