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LETTER

Pressure-induced transformations in kaolinite

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ABSTRACT

The compressional behavior of kaolinite (space group *C*1) from Keokuk, Iowa, has been studied to 7.8 GPa under static compression by synchrotron X-ray powder diffraction. Two phase transformations occur at ~3.7 (kaolinite-I/II) and ~7 GPa (kaolinite-II/III) that are registered by major changes in diffraction patterns. The layer shift involved in the I/II transformation preserves hydrogen-bonded contacts across the interlayer. This transformation removes cross-interlayer Al-Si superpositions and is analogous to the low-/high-dickite transformation, which occurs at ~2.6 GPa (Dera at al. 2003). The 7 GPa transformation from kaolinite-II to "kaolinite-III" involves considerable contraction of the *a*-*b* plane (2.5%), marked shortening normal to the polyhedral layers, and a volume contraction of about 3%. Comparison of experimental patterns of kaolinite-III with those calculated for non-standard polytypes predicted by ab initio methods to 60 GPa by Mercier and Le Page (2009) allows the identification of kaolinite-III with their high-pressure, one-layer Model 18 polytype. Kaolinite-III can be quenched to room pressure, although significant transformation to kaolinite-I was observed at 0.5 GPa on decompression. At ambient conditions kaolinite-III is 6% more dense than kaolinite-I, nacrite, and low-dickite. Elastic moduli for kaolinite-I and kaolinite-III have been obtained that indicate that kaolinite-III is more compressible than kaolinite-I, due primarily to in-plane (**a-b**) softening. Both high-pressure polytypes encountered experimentally were predicted ab initio to be strong candidates for high-pressure structures by Mercier and Le Page (2008, 2009). This agreement between experimental and ab initio studies is encouraging for the application of ab initio methods to complex polytypic systems.

Keywords: Kaolinite, high pressure, transformations, polytypism