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Anomalous behavior at the *I*2/*a* to *Imab* phase transition in SiO_2-moganite: An analysis using hard-mode Raman spectroscopy

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Abstract

The silica polymorph moganite is commonly intergrown with quartz in microcrystalline silica varieties that are less than ~100 Ma in age. Synchrotron X-ray diffraction suggests that a displacive phase transition occurs when moganite is heated above ~570 K, with an increase in symmetry from *I*2/*a* to *Imab*. In the present study, we employed hard-mode Raman spectroscopy to confirm the existence of the α-β moganite transformation and to offer complementary insight into the transition mechanism. Our analysis of the displacement of the 501 Δcm^{-1} symmetric stretching-bending vibration (B_{3g} mode) with changing temperature strongly supports the existence of a monoclinic-to-orthorhombic phase transition between 570 and 590 K. Between 593 and 723 K, however, the mode remained fixed at 496 Δcm^{-1}. This behavior was repeated on cooling, but with a hysteresis of over 100 K. We offer three hypotheses that may explain this observation: (1) the intergrowth of nanoscale quartz lamellae within moganite may exert a strain that inhibits the transition; (2) the transition may exhibit a martensitic character marked by the co-existence of α- and β-moganite over a finite temperature interval; and (3) the α- and β-moganite transition may occur via an intermediate phase.

Keywords: Moganite, phase transition, Raman spectroscopy, silica