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High-temperature structural change and microtexture formation of sillimanite and its phase relation with mullite

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Abstract

Synchrotron powder X-ray diffraction (XRD) experiments and transmission electron microscopy (TEM) observations of heat-treated sillimanite at various pressures were conducted to clarify the detailed phase relation between sillimanite and mullite. Under TEM, heat-treated sillimanite frequently showed anti-phase boundary (APB)-like textures with a displacement vector of $\frac{1}{2}[001]_{sil}$. Additional scanning TEM energy-dispersive X-ray spectroscopy analysis of regions with APB-like texture showed that they were clearly enriched in Al and accompanied by very fine, Si-rich glass inclusions, which indicates that the APB-like textures are composed of fine mullite. Moreover, synchrotron XRD patterns of these samples clearly showed double peaks of newly formed mullite and remnant sillimanite, indicating that the compositional transformation from sillimanite to mullite and glass is discontinuous. We separately determined the cell parameters of the sillimanite and mullite from the XRD pattern and found that the *b* axial length of the sillimanite increased with the treatment temperature, reflecting disordering of tetrahedral Al and Si in the sillimanite. In contrast, the positions of the deconvoluted mullite peaks indicated that the *a* axial length of mullite decreased as experimental pressure increased, owing to enrichment of the Si component. By projecting the cell parameters onto the *a*–*b* axial plane, the detailed changes in the crystallographic state of the sillimanite and mullite could be easily and comprehensively identified. On the basis of our results, we propose a new *P*-*T* diagram for the Al_2SiO_5 system that shows the transformation boundary between sillimanite and mullite + SiO_2-rich melt and the contour of the Al/Si order parameter of sillimanite.

Keywords: Sillimanite, mullite, high-temperature phase relation, TEM observation, synchrotron X-ray experiment