High-Temperature Structural Change of Sillimanite and Its Phase Relation with Mullite

We conducted high angular resolution powder X-ray diffraction experiments for sillimanite (Al2SiO5) heated at various temperatures and pressures in order to clarify its high-temperature phase relation with mullite (Al2[Al2+2xSi2−2x]O10–x). The results showed that sillimanite continuously transforms to mullite in composition by high-temperature annealing, and the cell parameters of remnant sillimanites indicated that tetrahedral Al and Si in sillimanite become continuously disordered as the annealing temperature is increased. Based on the results, we proposed a new P–T diagram of the Al2SiO5 system for geological applications.

Figure 1(b) shows representative XRD patterns obtained in this study. We successfully distinguished peaks of newly formed mullite and remnant sillimanite.

Figure 2: (a) Cell parameters of sillimanite and mullite against annealing temperature. The c axis of mullite is treated as twice the length to simplify the comparison with sillimanite. (b) P–T diagram of Al2SiO5 with the results of this study. The mullitization boundary and the contour of Q values determined by [7] are also shown. In the stability region of mullite + liquid, the Q values are shown for metastable sillimanite. Red open circles indicate that mullite is present, and green filled circles indicate that it is absent. Half-filled circles indicate that the presence of mullite is slight or unclear. The mullitization temperature at 1 atm (1300°C) determined by reaction kinetics analysis [8] is plotted by a red filled circle.

In contrast to the annealing temperature, the annealing pressure does not significantly affect the changes in cell parameters. The right panels of Fig. 2(a) show that the cell parameters of the sillimanite annealed at 0.2–2.5 GPa change with annealing temperature similarly to those of the sillimanite annealed at 1 atm. The degree of Al/Si order in sillimanite (Q) is almost independent of the imposed pressure.

REFERENCES