

Al/Si disordered anorthite in anorthite megacryst from Miyake-jima: effect of non-stoichiometry on Al/Si distribution

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The crystal chemistry of anorthite with the low content of albite (An_{92.0}Ab_{3.4}), part of a rapid cooled, anorthite megacryst occurring in 1940 ejecta from Miyake-jima volcano, Japan, has been investigated using single-crystal X-ray diffractometer and electron microprobe analyzer with wavelength dispersive X-ray spectroscopy (EMPA-WDS). The structure was refined in space group P-1 and cell parameters, $a = 8.182(6) \text{ \AA}$, $b = 12.883(4) \text{ \AA}$, $c = 7.092(4) \text{ \AA}$, $\alpha = 93.19(4)^\circ$, $\beta = 115.91(4)^\circ$, $\gamma = 91.18(4)^\circ$. The final weighted R-factor is 3.77 % for 1549 reflections. Averaged T-O distances are 1.681 \AA for T1(0), 1.674 \AA for T1(m), 1.677 \AA for T2(0) and 1.680 \AA for T2(m), indicating each Al occupancy of 0.501, 0.453, 0.472, and 0.496, respectively. These results suggest that the Al/Si-distribution in the tetrahedral framework is highly disordered (QOD = 0.06), which results in having the c-axis in half along that determined in Al/Si ordered anorthites ($c \sim 14 \text{ \AA}$).

Keywords: Anorthite, Al/Si order-disorder, Anorthite megacryst, Structural heterogeneity