Structures of High Temperature Ca-rich Plagioclase Feldspar – A Single-Crystal Neutron and X-ray Diffraction Study

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Plagioclase feldspar, the most common rock forming mineral in the Earth's crust, is a complete solid solution between albite (Ab: $NaAlSi_3O_8$) and anorthite (An: $CaAl_2Si_2O_8$) at high temperature. A better understanding of the $I\bar{1}$ structures of high temperature Ca-rich plagioclase feldspar clears the road to solid solution system. The $I\bar{1}$ structures of four natural Ca-rich plagioclase feldspars formed at high temperature were analysed using single-crystal neutron and X-ray diffraction. The neutron time-of-flight Laue diffractometer at the ORNL Spallation Neutron Source combined with single-crystal X-ray diffraction instrument was able to reveal some new details about these already intensively studied structures. The split oxygen atoms refined from the neutron diffraction data shows the underlying mechanism of the anisotropic $P\bar{1}$ ordering along ***c***-axis. The compositional ranges covered by the samples studied are quite rare for the $I\bar{1}$ structures. The incommensurately modulated *e*2 structure of some plagioclase samples can be easily confused with an $I\bar{1}$ structure from the diffraction pattern, which takes some previous published $I\bar{1}$ structures into question. An incomplete phase diagram for Ca-rich plagioclase feldspar is proposed to explain the rareness of the $I\bar{1}$ structure in this compositional range, and a time-temperature-transformation diagram for composition ~An_{66} is provided accordingly. The short-range $P\bar{1}$ ordering would still appear in plagioclase as sodic as An_{66}. The ordering can propagate along ***c***-axis via strongly bonded tetrahedral framework, and are weakly connected across ***c***-chains through the positional ordering of M sites that are loosely bonded to the oxygen atoms in the framework. The +1 charge of Na cation, compared to the +2 charge of Ca, is likely the reason why introducing albite content in anorthite structure would dramatically weaken the $P\bar{1}$ ordering.

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