Study on structure variations of incommensurately modulated labradorite feldspars with different cooling histories

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ABSTRACT

The incommensurately modulated structures of three intermediate plagioclase feldspars with compositions of ~An\textsubscript{51} are determined by single-crystal X-ray diffraction analyses. The samples selected cover a range of different cooling rate, from relatively fast to extremely slow. The structures show various ordering states that are directly correlated with the cooling histories of the samples. The slowest cooled sample shows an e1 structure with strong density modulation, along with nanoscale exsolution lamellae. The fastest cooled sample displays an e2 structure, without second-order satellite reflections (f-reflections) and density modulation. The sample with intermediate cooling rate shows a less ordered e1 structure with weak density modulation, but the modulation period and orientation are the same as in e2 structure. The comparison of the structures with the same composition reveals the ordering process and phase transitions during the cooling of plagioclase within the compositional range of Böggild intergrowth. New parameters from modulation waves can be used for quantifying the ordering state of plagioclase feldspars. Proposed phase relationship and T-T-T diagram for ~An\textsubscript{51} plagioclase feldspars are illustrated for explaining the relationship among CT, e1 and e2 structures, and relative cooling rates of their host rocks.

Keywords: Labradorite, incommensurate, modulated structure, density modulation, gabbro, e-plagioclase, cooling rate, ordering state, exsolution lamellae, intermediate plagioclase

INTRODUCTION

Plagioclase feldspar (Ca\textsubscript{x}Na\textsubscript{1–x}Si\textsubscript{3}−xAl\textsubscript{x}O\textsubscript{8}), a coupled solid solution between albite (NaAlSi\textsubscript{2}O\textsubscript{6}) and anorthite (CaAl\textsubscript{2}Si\textsubscript{2}O\textsubscript{8}), is the most abundant group of minerals in the Earth’s crust. The intermediate labradorite feldspars (An\textsubscript{50}−An\textsubscript{70}) are common in mafic rocks. Plagioclase with composition between ~An\textsubscript{25} to ~An\textsubscript{50} often show satellite diffractions (e-reflections) surrounding the absent b-reflections, indicating an incommensurately modulated structure (Bown and Gay 1959; Ribbe 1983a; Smith and Brown 1988). The aperiodic structure of intermediate plagioclase at low temperature and its complicated subsolids phase relations have puzzled mineralogists and petrologists for more than 70 years. Many structure models of the aperiodic structure have been proposed and refuted since the discovery of aperiodic plagioclase (Chao and Taylor 1940). Recent Z-contrast imaging study indicates polarity of the structure in a bytownite sample by Xu (2015), and is confirmed by a high-quality structure refinement of a metamorphic labradorite sample by Jin and Xu (2017). The structure of e-plagioclase is composed of periodic I1 like domains connected by inversion twin boundaries, instead of I\textsubscript{T} domains related by antiphase boundaries.

Incommensurately modulated structures are quite common in nature, and have been an important subject of crystallography for a long time. The modulated structure consists of a lattice periodic basic structure and a periodic modulation (Janssen et al. 2007). The structure of each unit cell of the basic lattice structure is modified by the modulation function from one to the next. The structure is incommensurate when the ratio between the modulation period and the basic unit-cell length is an irrational number. As the modulation function would never meet the basic lattice structure at the same point, the whole structure becomes aperiodic. The aperiodicity would be reflected in reciprocal space by satellite reflections that cannot be indexed with three integer numbers. An extra dimension has to be introduced for describing incommensurately modulated structure, where each parameter of the structure (occupancies, coordinates) is described by a periodic function. Characterization of incommensurately modulated structure in (3+1)D space is a fully developed theory (van Smaalen 2007; Wagner and Schoenleber 2009), and powerful and user-friendly software is available (Petőiček et al. 2014).

Despite recent studies, many questions about the phase relations remain unsolved. The incommensurately modulated plagioclase, or e-plagioclase, has been categorized into two types, e1 and e2, based on the existence of second-order satellite reflections, or f-reflections (Ribbe 1983b; Smith 1984; Carpenter 1994; McConnell 2008). In the diffraction pattern of an e1 structure, not only can the e-reflections surrounding the absent b-positions be observed, but also second-order satellite reflections, f-reflections appear around the main a-reflections; whereas in e2 structure, only the first-order satellites, e-reflections are present. Almost all previous samples studied by single-crystal X-ray diffraction were e1 with observable f-reflections. Little is known about the other category, the e2 structure, since only one structure refinement was done on this structure (Steurer and Jagodzinski 1988). The e1 structure is normally believed to only exist in the Ca-rich plagioclase (Ribbe 1983b; Smith 1984; Smith and Brown 1988), but Xu et al. (2016) discovered a plagioclase sample with a composition of ~An\textsubscript{45} that displays e1 structure, which makes the case more complicated. It was proposed that the CT ⇔ e2