American Mineralogist, Volume 102, pages 21–32, 2017

Solved: The enigma of labradorite feldspar with incommensurately modulated structure

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Abstract

Intermediate plagioclase feldspars are the most abundant minerals in the Earth's crust. Their incommensurately modulated structure has puzzled geologists and crystallographers for decades since the phenomenon in a labradorite was reported in 1940. Solving the structure is a necessary step toward mapping the complex subsolidus phase relations of plagioclase solid solution. The structure of a homogeneous labradorite (An_{51}) single crystal from a metamorphic rock is solved and refined from single-crystal X-ray diffraction. The result structure can be simplified as alternating $I1$-like lamellae domains related by inversion twins. The inversion boundary shows an anorthite-like structure with $I\bar{1}$ symmetry and is richer in Ca than the neighboring domains with opposite polarity. No albite-like subunits appear in the *e*-plagioclase structure. The modulated structure displays a unique Al-Si ordering pattern. A density modulation with a variation of 17 mol% in composition is also observed and can be properly described only by applying second-order harmonic waves for the atomic modulation functions. The modulated structure reveals details that cannot be observed from refinement with only main reflections and may be used to assess the ordering state and cooling rate of its host rock. The homogeneity of the crystal indicates the closure of the solvus for Bøggild intergrowth at low temperature. The highly ordered modulation supports the thermodynamic stability of *e*-plagioclase. Both Al-Si ordering and Ca-Na ordering are the driving force for formation of the incommensurately modulated structure.

Keywords: Intermediate plagioclase, incommensurate, modulated structure, density modulation, single-crystal XRD, *e*-plagioclase, labradorite, aperiodic crystal, Invited Centennial article