American Mineralogist, Volume 109, pages 1292–1302, 2024

Local strain heterogeneity associated with Al/Si ordering in anorthite, $CaAl_2Si_2O_8$, with implications for thermodynamic mixing behavior and trace element partitioning in plagioclase feldspars

Alison J. Atkinson[1], Tiziana Boffa Ballaran[2], and Michael A. Carpenter[1,*]

[1]Department Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.
[2]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany

Abstract

Hard Mode IR powder absorption spectroscopy has been used to characterize local strain relaxation associated with Al/Si ordering in a suite of synthetic anorthite samples with structural states that vary from a high degree of Al/Si order through a metastable incommensurate structure at intermediate states of order to long-range order with $I\bar{1}$ symmetry. The dominant feature accompanying the changing structural states is line broadening, which has been quantified by autocorrelation analysis and is attributed to local heterogeneous strain variations on a length scale of at least 1–5 unit cells. The autocorrelation results are consistent with contributions to the line broadening as being due to order parameters for both the $C\bar{1} \rightarrow I\bar{1}$ and $I\bar{1} \rightarrow P\bar{1}$ transitions, which couple biquadratically, $\lambda Q_{od}^2 Q_{displ}^2$. Close correlation with enthalpy variations from previously published calorimetric data indicates that the driving force for ordering can be understood in terms of elimination of strain fields arising from accommodating more or less rigid AlO_4 and SiO_4 tetrahedra in the feldspar framework. The metastable incommensurate structure of anorthite is closely analogous to the stable incommensurate structure that develops at intermediate compositions in the plagioclase solid solution, confirming that the same strain relaxation mechanism dominates the properties and behavior of all structural states across the solid solution. Elimination of strain heterogeneity by ordering on the basis of $I\bar{1}$ symmetry determines the form of non-ideal mixing shown by the solid solution at high temperatures, and changes in elastic properties may contribute to a break in the slope of partitioning of trace elements between crystals and melt.

Keywords: Anorthite, Al/Si ordering, hard mode IR spectroscopy, local strain heterogeneity, enthalpy