Thermal expansion of minerals in the pyroxene system and examination of various thermal expansion models

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Abstract

To examine the effects of chemical composition on thermal expansion in the pyroxene mineral group, X-ray diffraction data have been collected from room temperature to ~925 °C on a chemically diverse group of 13 pyroxenes including four orthorhombic and nine monoclinic samples. Additionally, resulting unit-cell volumes computed from the XRD data have proven to be good tests for a large number of thermal expansion models; the physical model by Kroll and coworkers and the empirical one by Fei have been found to be especially useful. Modeling also has allowed the connection of present data, collected at temperatures above 25 °C, to the volume data of other workers for much lower temperatures, well below 0 °C, and also extrapolation of values for volume and thermal expansion well beyond the measurement range.

We have found for orthopyroxenes that Fe2+-Mg2+ substitution has little effect on thermal expansion coefficients for volume. For clinopyroxenes, however, greater thermal expansion occurs in Ca2+ (diopside, augite, hedenbergite, johannsenite) than in Li+ (spodumene) or Na+ -bearing members (jadeite, aegirine, kosmochlor). Present data support the observation that differences in volume thermal expansion relate primarily to differences in expansion along the b crystallographic axis. This apparently is due to the greater concentration of M1 polyhedra along the b crystallographic axis, where expansion differences can be related to the shared O1-O1 polyhedral edge and inter-oxygen repulsion that is made easier by divalent, as opposed to trivalent, cation occupancy of the M1 crystallographic site.

Keywords: Pyroxenes, thermal expansion, modeling

Introduction

A principal line of research at Lafayette College over more than 20 years has been the investigation of the relationship of thermal expansion to the chemical compositions of minerals within specific structural groups. Previously published results include investigation of the entire feldspar system (Hovis et al. 1999, 2008, 2010; Hovis and Graeme-Barber 1997), nepheline-kalsilite feldspathoids (Hovis et al. 2006, 2003), and both F-Cl and F-OH apatites (Hovis et al. 2014, 2015). We now have expanded this work by collecting data on more than 50 mineral specimens covering wide compositional ranges in five additional silicate mineral systems. In the present paper, we explore thermal expansion relationships among pyroxenes.

A primary goal of present and previous work has been to provide valuable research experiences for undergraduate students at Lafayette College. Participants in the present work, now all graduated, are coauthors of this paper. The analysis of thermal expansion data has progressed significantly in the last decade, going far beyond questions asked in the previous studies listed above. In fact, high-quality volume-temperature (V-T) data can be utilized to test various mathematical formulations of V-T data and also incorporated into thermodynamic databases for the purpose of calculating phase equilibria at elevated temperatures. Even though pyroxene thermal expansion has been studied previously (references appropriate to specific minerals given later), an exploration of physical thermal expansion models for a systematic collection of pyroxenes is lacking. The current study provides data that can be used for such a purpose, similar to studies on plagioclase and olivine by Tribaudino et al. (2011) and Kroll et al. (2012), respectively.

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