High-pressure behavior of space group $P2/n$ omphacite

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ABSTRACT

A single-crystal X-ray diffraction (XRD) study, using a diamond-anvil cell at high pressure and room temperature, was performed on a crystal from a natural space group $P2/n$ omphacite sample with composition very close to Jd$_{27}$Di$_{18}$ and with a high degree of order in cation distribution. Unit-cell parameters were determined at 13 different pressures up to about 7.5 GPa. A third-order Birch-Murnaghan equation of state (BM3-EoS) fitted to the $P-V$ data yielded $V_o = 421.43(4)$ Å$^3$, $K'_{0} = 122(1)$ GPa, and $K'' = 5.1(3)$. The $K_{0}$ value for this sample lies between the data obtained for the two end-members jadeite and diopside, and describes a slight positive curvature trend.

During the same experiment, intensity data were collected and crystal structures were refined at 5 pressures up to 7.3 GPa. Both M1 and M2 polyhedra volumes showed a slight but significant change in slope at about 4 GPa. This behavior can likely be explained in terms of tilt angle variation of $TA$ and $TB$ tetrahedral, which also showed a change in slope with pressure, rather than in terms of bond length compression anomaly.

Keywords: Pyroxene, omphacite, high pressure, single-crystal XRD, crystal structures, diamond-anvil cell, equation of state

INTRODUCTION

Many recent X-ray diffraction studies have focused on the behavior under high-pressure conditions of clinopyroxene with different compositions (Downs 2003; Origlieri et al. 2003; Thompson et al. 2005; Bindi et al. 2006; McCarty et al. 2008; Nestola et al. 2005, 2006, 2007, 2008a, 2010; Gavrilenko et al. 2010). This is likely due to the very wide range of geological high-pressure environments in which this mineral is found, from metamorphic rocks to meteorites, and also as inclusions in diamonds (e.g., Nestola et al. 2007; Koch-Müller et al. 2004).

In particular, clinopyroxenes are very abundant in the upper mantle, and most mineralogical and geophysical investigations have concentrated on shedding light on the extremely complex geodynamic processes occurring at that depth (e.g., Agee 1999). Knowledge of the compressional and thermal behavior of clinopyroxenes is fundamental for understanding the geological environments in which these silicates play a crucial role. Concerning the high-pressure behavior of Na-clinoptyroxene, X-ray diffraction studies have been performed both on jadeite, aegirine, and hedenbergite end-members and on jadeite-aegirine and jadeite-hedenbergite solid solutions (Nestola et al. 2006, 2007, 2008a).

The compressional behavior of omphacite (solid solution between CaMgSi$_2$O$_6$, Di–NaAlSi$_2$O$_6$, Jd, end-members) was investigated for the disordered phase with space group $C2/c$ by McCormick et al. (1989) by single-crystal X-ray diffraction and by Nishihara et al. (2003) using an in situ multi-anvil apparatus by X-ray synchrotron radiation. The ordered phase with space group $P2/n$, was studied by Pavese et al. (2001) on powder material by X-ray synchrotron radiation. However no studies on the structural behavior at high pressure have been performed thus far on this mineral. The aim of this work is to define for the first time the crystal-structure evolution as a function of pressure and the pressure–volume equation of state for a natural ordered omphacite of space group $P2/n$ with low-Fe content by single-crystal X-ray diffraction (SCXRD). This work is part of a wider project focused on the high-pressure and high-temperature behavior of natural and synthetic Na-bearing pyroxenes.

EXPERIMENTAL METHODS

Sample

The sample investigated at high pressure in this work comes from the same crystal suite studied by Boffa Ballaran et al. (1998) and is labeled as their sample 74AM33. The chemical analysis of this sample is reported in Table 1. The sample was selected for its very low-Fe content to avoid the effect of iron on the Di-Jd solid solution. This sample also presents the highest degree of order for a natural omphacite among the samples studied by Boffa Ballaran et al. (1998). From this sample we picked out a single crystal, labeled N.4, suitable for the high-pressure experiments due to its sharp optical extinction, sharp diffraction profiles, absence of twinning and evident defects and appropriate crystal size (0.17 × 0.12 × 0.05 mm).

Chemistry

Chemical analysis was performed on the same crystal used for the high-pressure test. After extracting the crystal from the diamond-anvil cell (DAC) it was embedded in epoxy resin and polished for electron microprobe analysis (EMPA), which was carried out at the Dipartimento di Geoscienze (University of Padova) using a CAMECA-CAMEBAX electron microprobe operating in wavelength-dispersive mode with a fine-focused beam (~1 μm diameter), an acceleration voltage of 20 kV and a beam current of 10 nA, with 10 s counting times for both peak and total background. X-ray counts were converted to oxide wt% using the PAP correction program supplied by CAMECA (Pouchou and Pichoir 1991). Standards, spectral lines, and analytical crystals used were: albite (NaK$_2$), TAP, wollastonite (Si, CaO, TAP), olivine (MgK$_2$, TAP), Al$_2$O$_3$ (AlK$_2$), TAP, Mn$_2$TiO$_4$ (MnK$_2$, LiF, TaKo, PET), Cr$_2$O$_3$ (CrK$_2$, LiF), Fe$_3$O$_4$ (FeK$_2$, LiF). The oxide wt% obtained by averaging 15 microprobe analyses are reported in Table 1.