Equation of State of Fe- and Al-containing Silicate Perovskite

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Introduction

Aluminum and iron oxides are present at a few mole percent in all proposed mantle compositions, such as pyrolite and piclogite. Under the pressure and temperature conditions of the lower mantle, all Al_2O_3 is believed to be incorporated into $(Mg,Fe)SiO_3$ perovskite, which is generally accepted to be the most dominant phase in the Earth's lower mantle. An accurate determination of its equation of state (EOS) is of fundamental importance for developing compositional and mineralogical models of the Earth's interior. The EOS of $(Fe,Mg)SiO_3$ perovskite has been measured extensively [1-3]. Current interest has been focused on the role of Al and Fe^{3+} substitutions in the perovskite structure. Indeed, in a recent study [4], the substitution of Al in the perovskite structure has been demonstrated to have a significant effect on its thermal and elastic properties. This new finding requires adjustments in other components to match the perovskite properties with seismic observations. The effects of the simultaneous presence of Fe^{3+} and Al on the EOSs of the perovskite phase may be important but are still unknown. In this study, pressure-volume-temperature (P-V-T) measurements were carried out on a perovskite specimen with ~4 mol% Al_2O_3 and 7 mol% FeO.

Methods and Materials

The perovskite sample studied in this work was synthesized from a mixture of synthetic crystalline othorpyroxene, $(Mg_{0.87}Fe_{0.13})SiO_3$, and glass containing 50 mol% $MgSiO_3$ and 50 mol% $Mg_3Al_2Si_3O_{12}$ $(En_{50}Py_{50})$ in the weight ratio 7:3. The experiment was conducted at ~26 GPa and 1873K for 24 h by using a 2000-ton uniaxial split-sphere apparatus at Stony Brook. X-ray diffraction indicates that the run product consists of a single-phase perovskite with trace amounts of majoritic garnet. X-ray diffraction experiments were conducted by using a DIA-type cubic anvil apparatus [5] and a T-cup high pressure system [6]. An energy-dispersive x-ray method was employed by using white radiation from the superconducting wiggler magnet at beamline X17B of the National Synchrotron Light Source and from the bending magnet at beamline 13-BM-D of the APS. In both experiments, NaCl was used as an internal pressure standard, and temperatures were measured by a W/Re25%-W/Re3% thermocouple.

The experiment reported here was carried out by the following procedures. We first compressed samples at room temperature to ~19 GPa. Heating to the maximum temperature of 873K followed. X-ray diffraction data were collected upon cooling to minimize the nonhydrostatic stress that built up during the room-temperature compression. The same procedure was repeated several times at lower pressures to obtain sufficient data at many different P-T conditions.

Results

The volume data have been obtained on perovskite at pressures up to 19 GPa and temperatures of 300, 473, 673, and 873K (Fig. 1). From these data, thermal and elastic parameters were derived from various approaches

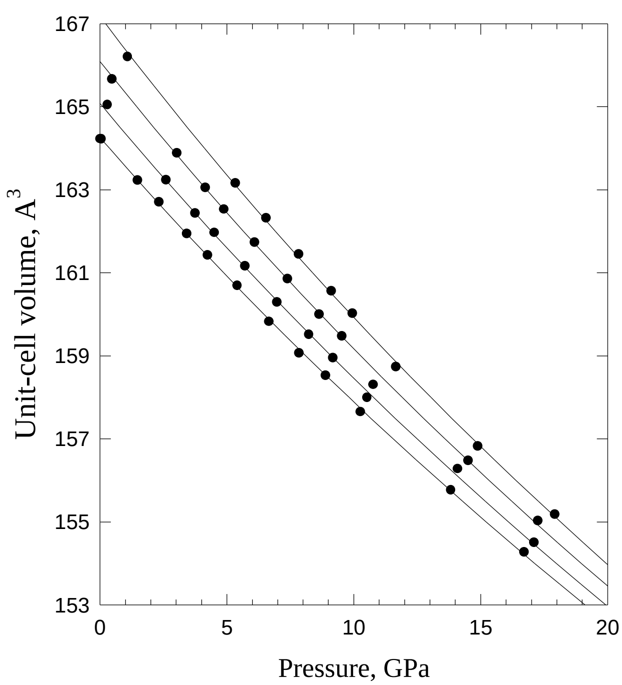

FIG. 1. P-V-T data for silicate perovskite containing ~4 mol% Al_2O_3 and 7 mol% FeO. The curves represent results of the least-squares fit by using the high-temperature Birch-Murnaghan EOS at various temperatures.

based on the Birch-Murnaghan EOS and on the relevant thermodynamic relations. The results from three different EOSs state are remarkably consistent. With $(\partial K_T/\partial P)_T$ fixed at 4 (which is nevertheless supported by the experimental data), we obtained K_0 = 234(2) GPa, $(\partial K_T/\partial T)_P$ = -0.048(6) GPa K^{-1}, $(\partial K_T/\partial T)_V$ = -0.025(4) GPa K^{-1}, and $a_T = 2.49(30) \times 10^{-5} + 1.02(\pm 0.53) \times 10^{-8} T$. The large $(\partial K_T/\partial T)_V$ value suggests that there is a strong dependence of thermal pressure on volume for Fe- and Al-containing silicate perovskite.

Discussion

The EOS parameters obtained from preliminary analyses of P-V-T data are similar to those reported for perovskite containing 5 mol% Al_2O_3. This infers that within the composition range of these studies, iron does not have a significant effect on the thermal and elastic properties of lower-mantle perovskite. Therefore, they are insensitive to the Fe-Mg partitioning between perovskite and magnesiowüstite, which would otherwise complicate the compositional models for the lower mantle.

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