Elasticity Systematics of $CaTiO_3$-$CaFeO_{2.5}$

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Introduction

Recent studies have shown that all Al_2O_3 is incorporated into (Mg,Fe)SiO_3 perovskite in the lower mantle conditions regardless of the mantle composition models (e.g., pyrolite and piclogite).[1] Equation of state study on Al-enriched silicate perovskite has shown that the presence of 5% Al_2O_3 has a significant effect on the elastic bulk modulus of the silicate perovskite.[2] *Ab initio* calculations suggested that oxygen vacancies in Al-bearing perovskites could explain the experimentally observed lower compressibility. However, there is no direct evidence indicating the preferred substitution mechanism for the incorporation of Al^{3+} into $MgSiO_3$ perovskite. Two mechanisms have been suggested.[3] The first mechanism is that Al^{3+} enters both cation sites, which does not require the creation of vacancies for charge balance. The second mechanism is that Al^{3+} replaces silicon only and that oxygen vacancies are required for charge balance.

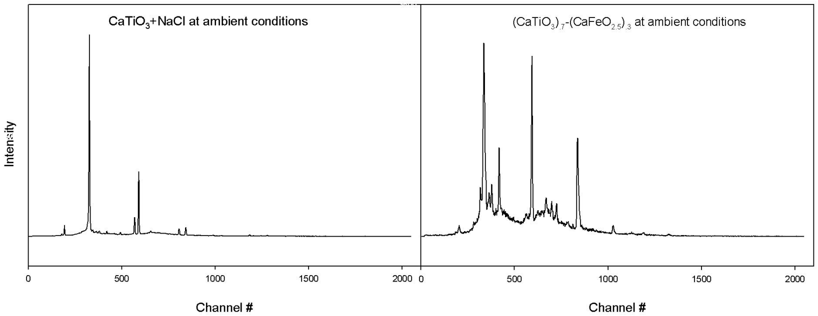

FIG. 1. Diffraction patterns of samples at ambient conditions.

In order to study the effects of oxygen vacancies on the equation of state of perovskite-structured phases in general, we would like to embark on the investigation of the $CaTiO_3$-$CaFeO_{2.5}$ perovskites. As shown in previous studies, this system exhibits a full range of possible defect concentrations and has been well characterized using x-ray diffraction, Mossbauer spectroscopy, and transmission electron microscopy.[4,5] The structural phenomena of $CaTiO_3$-$CaFeO_{2.5}$ perovskites, along with the variation of composition and temperature, have been described as short-range and long-range order of oxygen vacancies, cation order-disorder, and displacive phase transition, all of which have influences on physical properties.[6] In this study, we would like to investigate the relationship between the compressibility of this suite of perovskites and the ordering of oxygen vacancy and cation order-disorder. This systematic study on the oxygen vacancy-bearing perovskites will bring insights into the elastic properties of mantle perovskite.

Methods and Materials

The samples of $(CaTiO_3)_X$-$(CaFeO_{2.5})_{1-X}$ used in this study were the compositions of X = 0 and 0.7. An energy-dispersive x-ray method was employed using white radiation to collect the cell parameters of sample and pressure caliber (NaCl used here) at beamline at sector 13-BM at high pressure and room temperature. High pressure was generated by using a 250-ton large-volume press at sector 13-BM. A 6 × 6 × 6 mm^3 cell assembly, which is a mixture of amorphous boron and epoxy resin, was used in this study. In order to compare the equation of state of two materials directly, we loaded two $CaTiO_3$ in the same high-pressure run. To do so, two teflon capsules were loaded in a boron epoxy cube. A liquid pressure medium (4:1 methanol:ethanol mixture) was used to provide the pseudohydrostatic conditions at high pressures.

Results

X-ray diffraction patterns of $CaTiO_3$ and $(CaTiO_3)_{.7}$-$(CaFeO_{2.5})_{..3}$ (Fig.1) were collected up to 6 GPa at room temperature. General structure analysis system (GSAS) is employed to analyze the x-ray diffraction data to get precise unit-cell parameters at experimental conditions. The data analysis is in progress.

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