Elasticity and Strength of $CaSiO_3$ Perovskite at Lower Mantle Pressures

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Introduction

Knowledge about the elastic tensor of deep earth materials is essential for understanding the radial and lateral variation of seismic velocities and seismic anisotropy. Yield strength is one of the most important but poorly understood mechanical properties of materials. Calcium silicate perovskite ($CaSiO_3$) is considered to be the third most abundant phase in the deep mantle [1], and its existence in natural samples has been inferred from $CaSiO_3$ compositions in diamond inclusions [2]. Furthermore, it is representative of the perovskite-structured materials containing silicon in sixfold coordination that are expected to dominate the deep mantle.

The elastic and rheological properties of $CaSiO_3$ perovskite are very poorly understood because it is not quenchable at ambient conditions. Available results on the elastic properties are restricted to analog [3] and theoretical studies [4]. In addition, theoretical studies [5] have predicted that a cubic-tetragonal transition may occur under lower mantle conditions, but no experimental evidence has been found for this yet. The equation of state (EOS) and stability of $CaSiO_3$ perovskite have been examined at conditions up to as high as 96 GPa and 2400K [6]

The measurement of the anisotropy of lattice strain due to nonhydrostatic compression can yield information on strength and elasticity under high-pressure conditions. We previously used this technique successfully to study a range of materials, including ringwoodite and stishovite at the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory and at the APS at Argonne National Laboratory [7-10]. Because of its cubic crystal structure, calcium perovskite is an ideal candidate for radial diffraction studies. Measurements to date conducted by using lattice strain theory and an axial x-ray geometry indicate that this silicate has an appreciable yield strength and/or elastic anisotropy and that this sensitivity to deviatoric stress likely explains discrepancies in the 300K EOS data for this material [10]. Here we report on the first measurements of the yield strength and elasticity of Ca-perovskite to lower mantle pressures by using radial x-ray diffraction.

Methods and Materials

The starting material for this study was a natural wollastonite ($CaSiO_3$) that was mixed with platinum and loaded into a 100-μm hole of a beryllium gasket. The sample was then compressed under intentionally nonhydrostatic conditions in a diamond anvil cell. A gold foil was placed at the center of the sample to serve as a pressure standard and positional reference. The samples were converted to $CaSiO_3$ perovskite at 15-20 GPa by laser heating, with Pt serving as the laser absorber. Energy-dispersive x-ray diffraction data were collected at beamline 13-BM-D of the GSECARS sector. Data were collected as a function of angle from the loading axis at each pressure step by using a radial geometry in the diamond cell. Spectra were collected only after a sufficient amount of time had elapsed to allow for stress relaxation in the sample.

Results and Discussion

Our diffraction patterns show that the lattice strain anisotropy for this material is large and readily measured (Fig. 1). As predicted by lattice strain theory, we observe a linear relation between the measured d-spacings and the parameter $1\text{-}3\cos^2\psi$, where ψ is the angle between the diffraction plane normal and the diamond cell loading axis (Fig. 2). The ratio of differential stress to shear modulus is 0.016 ± 0.005 to 0.039 ± 0.004 for $CaSiO_3$ perovskite at pressures up to 61 GPa. These values are similar to those found for stishovite [7] but generally lower than those found for four-coordinated silicates such as ringwoodite [8]. The yield strength of Ca-perovskite increases from 3 to 10 GPa over a pressure range from 19 to 61 GPa. Systemtatic trends for six-coordinated silicates allow us to predict the room-temperature strength of $MgSiO_3$ perovskite, and the results are in good agreement with recent micro strain experiments. The hydrostatic EOS inferred from the measured lattice strains is consistent with other experiments. Single-crystal elastic constants for $CaSiO_3$ perovskite are in agreement with theoretical calculations [4] and indicate that elastic anisotropy decreases with pressure. The presence of a possible phase transition in $CaSiO_3$ perovskite may explain differences between our study and some previous axial diamond cell experiments.

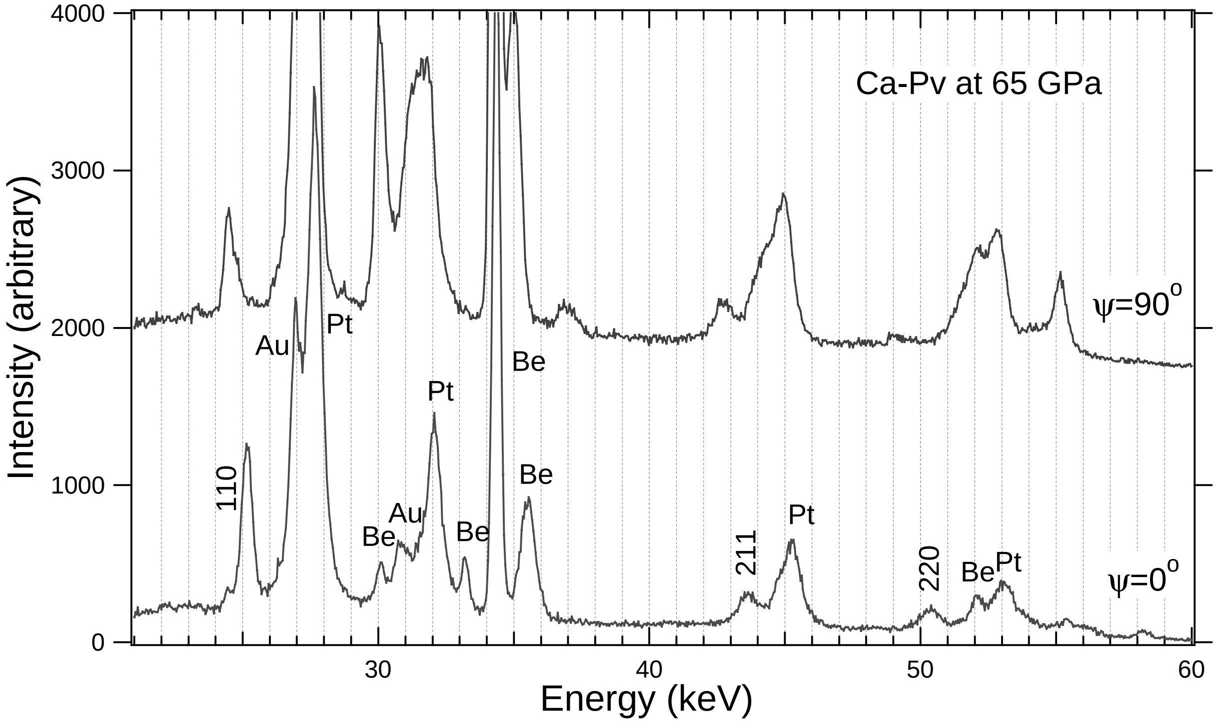

FIG. 1 Representative spectra of $CaSiO_3$ perovskite phase obtained at 65 GPa by using radial x-ray diffraction in the diamond anvil cell. The lower spectrum is the maximum strain direction, and the upper spectrum is the minimum strain direction. The sample peaks are labeled with Miller indices; other peaks arise from gold, platinum, and beryllium.

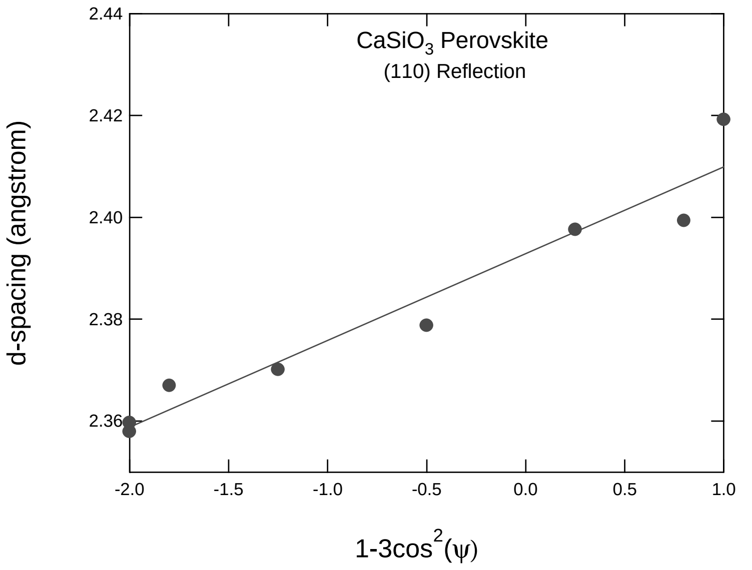

FIG. 2. Variation of d-spacing of the (110) reflection of $CaSiO_3$ perovskite as a function of angle from the loading axis of the diamond cell.

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