

## Equation of state of CAS phase to 44 GPa at 300 K

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### Introduction

The calcium aluminosilicate (CAS) phase,  $\text{CaAl}_4\text{Si}_2\text{O}_{11}$ , occurs in rocks formed from sediments at pressures corresponding to those found in the upper mantle and transition zone conditions. Previous studies reported that this CAS phase has a hexagonal barium ferrite-type structure. The physical properties of a given phase in the subducted sediments may affect the dynamics of the subduction and material circulation in the mantle and, therefore, it is important to determine the compressibility of the CAS phase.

### Experimental methods

High-pressure X-ray diffraction experiments were performed using a laser-heated diamond anvil cell (LHDAC) high-pressure apparatus. The powdered CAS phase,  $\text{CaAl}_4\text{Si}_2\text{O}_{11}$ , was loaded into a 100  $\mu\text{m}$  diameter hole that was drilled into a rhenium gasket. Platinum powder was mixed with the sample to absorb the laser radiation to provide a heat source, and was also used as an internal pressure calibrant. Argon was used as a pressure transmitting medium to reduce deviatoric stress and temperature gradients in the sample. The samples were heated with a YAG laser to overcome any potential kinetic effects on possible phase transitions. The pressure was determined from the observed unit cell volume of platinum using the Pt equation of state. The samples were probed using an angle-dispersive X-ray diffraction technique at the synchrotron beam lines BL13A, Photon Factory in Japan [1]. A monochromatic incident X-ray beam with a wavelength of about 0.42 angstrom was used. The X-ray beams were collimated to a diameter of 30  $\mu\text{m}$ , and the angle-dispersive X-ray diffraction patterns were obtained on an imaging plate (Rigaku).

### Results and Discussion

The powder X-ray diffraction data of the CAS phase at ambient pressure revealed that it had a hexagonal barium ferrite-type structure ( $P6_3/mmc$ ), with unit cell dimensions of  $a = 5.428(4)$   $\text{\AA}$  and  $c = 12.728(26)$   $\text{\AA}$ . The volume and density of the CAS phase at ambient pressure were  $324.7(8)$   $\text{\AA}^3$  and  $3.888(10)$   $\text{g/cm}^3$ . Our sample was heated using the laser after each pressure increment, and the X-ray diffraction measurements were taken. The laser heating annealed the sample, and reduced any pressure gradient occurring across the sample, thus improving the quality of the X-ray diffraction data. The heating was performed at pressures  $> 15$  GPa, which corresponds to the stability field of the CAS phase, because we investigated the possibility that the CAS phase would

dissociate into separate phases under metastable conditions. The entire sample was carefully heated by scanning with the laser beam to eliminate any potential reactions with either the argon pressure transmitting medium or the platinum pressure calibrant. The effect of pressure on the volume of the CAS phase is plotted in Fig. 1. The P-V data were fitted to the Birch-Murnaghan equation of state to determine the elastic parameters:

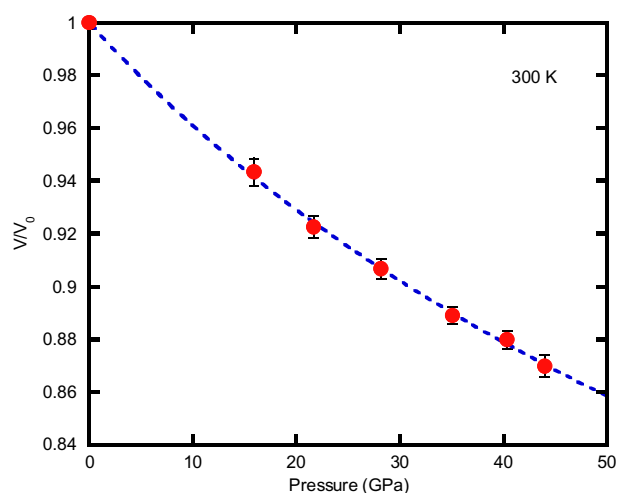
$$P = 1.5K_0(x^{-7}-x^{-5})[1+0.75(K_0'-4)(x^2-1)]$$

where  $x = (V/V_0)^{1/3}$ ; and  $V_0$ ,  $K_0$ , and  $K_0'$  are the volume, the isothermal bulk modulus, and the first pressure derivative of the isothermal bulk modulus, respectively. The isothermal bulk modulus and the first pressure derivative of the isothermal bulk modulus were determined to be  $K_0 = 229(9)$  GPa and  $K_0' = 4.7(7)$ , respectively [2]. When the value of  $K_0'$  was set to  $K_0' = 4$ , then a value of  $K_0 = 239(2)$  GPa was obtained. We did not observe any phase transition occurring in the CAS phase up to a pressure of 44 GPa, which was the maximum pressure used in this study.

### References

- [1] Ono et al., J. Appl. Phys. 97, 073523 (2005).
- [2] Ono et al., Phys. Earth Planet. Inter. 150, 331 (2005).

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**Figure 1.** Pressure-volume data for the CAS phase at 300 K. Dashed curve: third-order Birch-Murnaghan equation fit with  $K_0$  and  $K_0'$  are 229 (GPa) and 4.7, respectively.