

Equation of State, Pressure Calibration and Sound Velocity Measurements on Wadsleyite to 20 GPa

B. Li,¹ J. Kung,¹ T. Uchida,² Y. Wang²

¹SUNY Stony Brook, Stony Brook, NY U.S.A.; ²Argonne National Laboratory, Argonne, IL U.S.A

Introduction

Seismic studies provide information about density, compressional (P) and shear (S) wave velocity profiles as a function of depth as well as their lateral variations as a function of depth[1]. An important feature is the 410 km discontinuity which has been attributed to the elasticity change associated with the olivine to wadsleyite phase transformation. Successful interpretation of the magnitude of this seismic discontinuity observed in seismic data has great significance in constraining the Earth's composition. In this report, we describe the results for a polycrystalline Mg_2SiO_4 wadsleyite from a simultaneous study of equation of state, pressure calibration, and sound velocities using combined synchrotron X-radiation and ultrasonic interferometry techniques. These techniques greatly extend our experimental studies on the elasticity of deep Earth materials towards the pressure and temperature conditions of the Earth's lower mantle.

Methods and Materials

The experimental facility installed at 13-ID-D/GSECARS for conducting the experiments described in this study. The key elements of this experimental set-up include the multi-anvil press, a solid state detector for X-ray diffraction, the X-ray imaging system consisting of a YAG crystal and a CCD camera, and the ultrasonic system. The multi-anvil system uses a Kawai

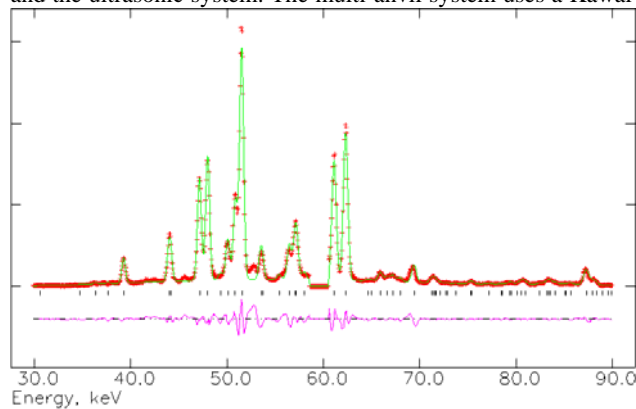


Fig. 1 X-ray diffraction pattern (cross) and fit (line)

type double-stage multi-anvil high-pressure module (T-25), compressed in a 1000-ton hydraulic press[2]. Pressure is generated in two stages, of which the first stage is composed of a uniaxial compression of the top and bottom guide blocks. The second stage consists of eight 25-mm edge length WC cubes, each has a corner truncated to a triangular face compressing an octahedral pressure transmitting medium (semi sintered MgO), which contains heating element and the sample. Potentially, a maximum pressure of ~ 30 GPa and 2500K in temperature can be achieved simultaneously for millimeter sized samples[2]. Details about the sample cell assembly can be found in [3].

X-ray diffraction data are collected using a solid state detector equipped with a multi-channel analyzer (MCA). The detector is mounted on a stage behind the press and is set at a

diffracting angle of 5.5 degree. The incident X-ray beam is collimated to 100 μm (vertical) by 200 μm (horizontal) to limit the diffracting volume. During the experiment, by moving the press to position the sample and the pressure standard at the diffracting center, X-ray diffraction from the sample and the pressure standard are recorded. A polycrystalline sample was hot-pressed using the 1000-ton Uniaxial Split-Cylinder Apparatus (USCA-1000) in the High Pressure Lab at Stony Brook at 15 GPa 1500K. Fig. 1 is an example of the recorded X-ray diffraction pattern at high pressure for a polycrystalline wadsleyite. A full profile fitting using GSAS package and the La Bail method yields unit cell parameters (therefore unit cell volume and density) [4].

Results and Discussion

The measurement has been conducted to $P \sim 20$ GPa at 300K.

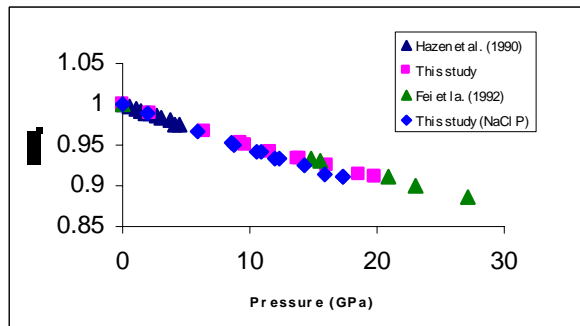


Fig. 2. Volume change of wadsleyite as a function of pressure. Data from [6] on iron bearing wadsleyite and iron free wadsleyite from [5] are also plotted. The squares are plotted against pressures determined from Decker's Eos for NaCl and diamonds are against pressures from finite strain calculation. The uncertainty in volume is $\sim 0.1\%$ and uncertainty in pressure is about 0.05 GPa.

In this experiment, the pressure was first increased to a designated peak value at room temperature and then the temperature was increased to about $\sim 673\text{K}$ to relax the deviatoric stress caused by solid pressure medium (NaCl+BN) surrounding the sample. After reaching the peak P and T conditions, the pressure was released slowly and data were also collected along decompression at room temperature. The sample recovered from this experiment remained its original length, suggesting that the surrounding NaCl provided a desired pseudo-hydrostatic stress condition; and the sample had only been subjected to elastic strain during the entire experiment. X-ray diffraction patterns of the sample showed the same peak widths during cold compression, heating as well as decompression of this experiment, suggesting that the intergranular stresses were very low. Analysis on relative peak position shift of NaCl at ~ 20 GPa at room temperature indicated the stress level was about 0.02GPa, which was within the resolution of the current set-up.

Fig. 2 summarizes the change of the unit cell volume as a function of pressure obtained from the current experiment. Within the experimental uncertainties, the data collected along compression and those along decompression after heating are indistinguishable. Comparing the unit cell volume change as a function of pressure with two previous studies, one on iron-free wadsleyite up to 4 GPa [5], and the other on wadsleyite with 16% iron content by [6] to 27 GPa, we found that all data below 5 GPa are compatible with each other if we consider the uncertainty in our pressure determination using Decker (1971) NaCl pressure scale (~3%). Beyond 5 GPa, however, the NaCl pressure deviates from the sample pressure independently determined using acoustic velocity and unit cell volume as illustrated in [3] by as much as ~12.0(1.2) % at the peak pressure. Current volume data as a function of sample pressure are in complete agreement with previous studies of [5] and [6] up to the peak pressure of this study.

From the travel times and the length data, P and S wave velocities at high pressures are obtained and plotted in Figs. 3. Previous acoustic data available for comparison include polycrystalline data to 12 GPa using ultrasonic technique of [7] as well as the single crystal results of Brillouin scattering in a diamond anvil cell by [8]. It is worth noting that in previous ultrasonic experiment of [8], the pressure was determined based on the observation of the phase transitions of Bi (2.55 GPa, 7.7 GPa) and ZnTe (12.0 GPa) enclosed in their acoustic experiment as internal pressure calibrants; in contrast to the direct determination using measured acoustic velocities and density data as described above. However, as seen in Fig. 3, these two data sets show a remarkable agreement in both P and S wave velocities. Current data also agree with previous Brillouin scattering data of [8] very well in which their pressure was determined using ruby pressure scale.

Finite strain analysis of current data following these procedures in [3] yields $K_{0S}=172$ (2) GPa, $K_0'=4.3$ (1), $G_0=110$ (1) GPa and $G_0'=1.5$ (1) when all data are used, while $K_{0S}=174$ (2) GPa, $K_0'=4.2$ (1), $G_0=111$ (1) GPa and $G_0'=1.5$ (1) are obtained if the datum point ~2 GPa is excluded from fitting due to the poor alignment of the sample in the X-ray image. These results compare well with values of $K_{0S}=175$ (2) GPa, $K_0'=4.0$ (1), $G_0=112$ (1) GPa, and $G_0'=1.4$ (1) which are obtained if the sample lengths derived from the unit cell volumes are used. The values in the parenthesis indicate one standard deviation. Compare with our previous measurements [9] on the same sample using combined ultrasonic and X-ray diffraction techniques to 7 GPa ($K_{0S}'=4.5$ $G_0'=1.5$), a gradual decrease in the pressure derivatives of bulk modulus is suggested. Current results on K_{0S} , K_0' , G_0 and G_0' are very consistent with studies at similar pressure range using ultrasonic method [7] and Brillouin scattering techniques [8]. When applying these new results to the modeling of the mantle composition, current study provides further supports that the upper mantle and transitions zone favors a pyrolytic composition as shown in [9].

Acknowledgement

This research was supported by National Science Foundation under grant EAR000135550 to BL. These experiments were performed at GeoSoilEnviroCARS (Sector 13), Advanced Photon Source (APS), Argonne National Laboratory. GeoSoilEnviroCARS is supported by the National Science Foundation - Earth Sciences (EAR-0217473), Department of Energy - Geosciences (DE-FG02-94ER14466) and the State of Illinois. Use of the APS was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Energy Research, under Contract No. W-31-109-Eng-38.

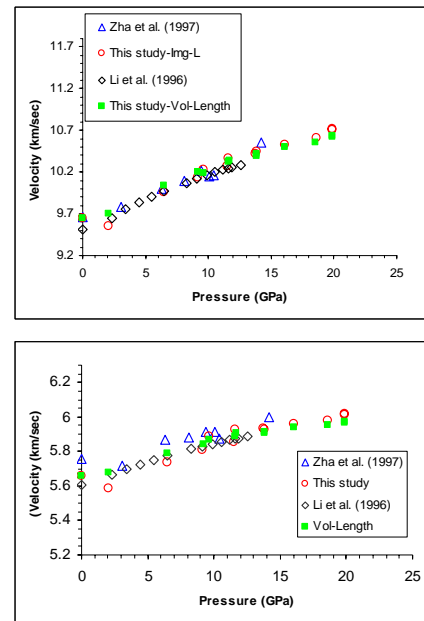


Fig. 3. Comparison of P and S wave velocities of wadsleyite from this study with previous measurements

References

- [1] G. F. Davis, A. M. Dziewonski, A.M., *Phys. Earth Planet. Interi.*, **10**, 336-343, (1975).
- [2] T. Uchida, Y. Wang, M. L. Rivers, S.R. Sutton, D.J. Weidner, M.T. Vaughan, J. Chen, B. Li, R. A. Secco, M. D. Rutter, H. Liu, 2002. *J. Phys. Condens. Matter*, **44**, 11517-11523 (2002).
- [3] B. Li., J. Kung, R. C. Liebermann. *Phys. Earth Planet. Interi.*, **143-144**, 559-574 (2004).
- [4] A. C. Larson, R. B. Von Dreele, 1988. Los Alamos Natl. Lab., Los Alamos, NM, Report LAUR 86-748.
- [5] R. M. Hazen, J. M. Zhang, J. Ko, *Phys. Chem. Miner.*, **17**, 416-419 (1990).
- [6] Y. Fei, H-K Mao, J. Shu, *J. Geophys. Res.*, **97**, 4489-4495 (1992).
- [7] B. Li, G. D. Gwanmesia, R. C. Liebermann. *Geophys. Res. Lett.*, **23**, 2259-2262 (1996).
- [8] C-S Zha, T. S. Duffy, R. T. Downs, H-K Mao, R.J. Hemley D. J., Weidner, in Manghnani, M.H., Yagi, T. (Eds), *American Geophysical Union*, Washington, DC, pp. 9-16 (1998).
- [9] B. Li, R. C. Liebermann, D. J. Weidner. *Science*, **281**, 675-677 (1998).