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Anhydrous Phase B: Transmission Electron Microscope Characterization and Elastic Properties

Patrick Cordier (1), Ahmed Addad (1), Philippe Carrez (1), Damien Jacob (1), Shun-ichiro Karato (2), Anwar Mohiuddin (2), Alexandre Mussi (1), Billy Nzogang (1), Pascal Roussel (3), and Andrea Tommasi (4)

(1) Univ. Lille, CNRS, INRA, ENSCL, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France, (2) Yale University, Department of Geology and Geophysics, New Haven CT 06520-8109, USA, (3) Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unite´ de Catalyse et de Chimie du Solide, F-59000 Lille, France, (4) Univ. Montpellier, CNRS, Geosciences Montpellier, F-34095 Montpellier, France

In this contribution we describe the Transmission Electron Microscope (TEM) characterization of transformation products resulting from annealing San Carlos olivine at 14 GPa, 1400 °C for 30 min in a KIWI 1000-ton Kawai-type multi-anvil apparatus installed at Yale University. TEM characterization was carried out at the University of Lille. TEM samples were prepared using the focus ion beam (FIB) technique. Two distinct high-pressure phases are found in the remaining olivine matrix in these thin foils. One is readily identified as wadsleyite. The other one appears as thin lamellae with some epitaxial relationships with olivine. The phase within these lamellae can be indexed neither as wadsleyite, nor as ringwoodite. The largest lamella was ca. 320 nm wide. Nevertheless, this allowed selected area electron diffraction to be performed. We used precession electron diffraction tomography to perform electron crystallography by sampling the reciprocal space through tilt series from -45° to +45° with an acquisition step of 1°. The analysed volume was < 0.025 μm3. The data were processed using the PETS program (Palatinus, 2011) to produce a complete representation of the reciprocal space. The program JANA2006 (Petříček et al., 2014) was afterward used to find the unit cell (a = 5.9181(13) Å, b = 10.1141(9) Å, c = 14.3428(13) Å, and V = 858.5(2) Å3). The structure was then solved ab initio using the charge flipping algorithm taking into account the chemical information provided by the EDS analysis (Mg1.99Fe0.21Si0.84O4). The structure refinement, using dynamical theory, yielded a model with some octahedrally-coordinated silicon. This coordination has been confirmed by performing energy loss near edge structure (ELNES) at the O K-edge. Finally, the crystallographic data obtained correspond to the anhydrous phase B (Anh-B) as first determined by Finger et al. (1989).
Ab initio calculations based on the density functional theory (DFT) were performed using the VASP simulation package to calculate the equation of state and the elastic constant tensor of Anh-b at 15 GPa. This information was used to predict the seismic properties of Anh-B in the mantle.
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