

Equation of state and high-pressure lattice behavior of CaCO_3 aragonite

YING LI^{1*,2}, YONGTAO ZOU², TING CHEN³,
XUEBING WANG³, XINTONG QI³, JIANGUO DU¹,
BAOSHENG LI²

¹ CEA Key Laboratory of Earthquake Prediction
(Institute of Earthquake Science), China
Earthquake Administration, Beijing, 100036,
China

² Mineral Physics Institute, Stony Brook University,
Stony Brook, NY 11794-2100, USA

³ Department of Geosciences, Stony Brook
University, Stony Brook, NY 11794-2100, USA

Corresponding to: Ying Li
(subduction6@hotmail.com)

P-V-T equation of state of aragonite was determined by in situ synchrotron X-ray diffraction experiments on a hot-pressed polycrystalline specimen of aragonite within its stability field up to 5.8 GPa and 1173 K. As a complement to this experimental study and to investigate the bond rotation and shortening, first principles density functional theory calculations were performed up to 20 GPa. Thermoelastic parameters for aragonite (CaCO_3) were derived by a least-squares fit of the experimental P-V-T data to the third-order Birch-Murnaghan equation of state (EOS), yielding the bulk modulus and its pressure and temperature derivatives $K_{T0} = 65.24 \pm 0.24$ GPa, $K'_{T0} = 4.95 \pm 0.12$, $(\partial K_T / \partial T)_P = -0.024 \pm 0.002$ GPa K^{-1} and volume thermal expansion $\alpha_{300} = (6.1 \pm 0.7) \times 10^{-5}$ K^{-1} . The analyses of the axial compressibility at ambient temperature show that the c-axis is much more compressible than the a- and b- axes. Based on first principles calculations, the anisotropic compression behavior of aragonite structure is explained by the heterogeneous shortening of $\langle \text{Ca-O} \rangle$ and $\langle \text{C-O} \rangle$ bond lengths and the rotation of $\langle \text{O-C-O} \rangle$ angles along the a-, b-, and c-axes, whereas the unit cell volume change of aragonite under compression is accommodated by comparable compression rate of the CaO_9 polyhedra and the voids in the crystal lattice. The results attained from this study provide important thermoelastic parameters for understanding the thermodynamic behavior and chemical reactions involving aragonite at subduction zone conditions.