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Structure and elasticity of wadsleyite at high pressures

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ABSTRACT

The athermal equilibrium structure, the equation of state, the elastic constants, and O atom charges were calculated for Mg_2SiO_4 wadsleyite over a range of pressures using a plane-wave pseudopotential method. The zero-pressure volume is 2% lower and the bulk modulus is 4.5% higher than experimentally observed. After correcting for zero point motion and the 300 K temperature difference between theory and experiment, using a Debye model, the calculated zero pressure volume is within 1% of experiment and the bulk modulus agrees within experimental error. The structure compresses anisotropically with linear moduli for the **a**, **b**, and **c** axes of 610 GPa, 599 GPa, and 454 GPa, respectively. The compression is largely taken up by the Mg octahedra M1, M2, and M3 which are much softer than the Si tetrahedra, with polyhedral bulk moduli of 161 GPa, 159 GPa, 157 GPa, and 331 GPa, respectively. The M1 and M3 octahedra were found to compress anisotropically which explains the greater compressibility of the **c** axis. The geometry of the Si_2O_7 group is characterized by a small Si-O-Si angle of 121.2°; compression of this group is largely accommodated by shortening of the Si-O bonds, while the inter-tetrahedral angle is almost pressure independent. We find that our results at ambient pressure are consistent with previously established systematics relating bulk modulus to volume, and Si-O-Si angle to Si-O bond length. However the variation of these quantities upon the application of pressure leads to trends that are distinct from the systematics. The calculated zero pressure elastic constants agree to within 10% with available Brillouin scattering data, with the exception of C_{12} which is 15% higher than experimentally observed. The calculated isotropically averaged bulk and shear modulus and their pressure derivatives are $K_0 = 182$ GPa, $K_0' = 4.23$, and $G_0 = 116$ GPa, $G_0' = 1.10$, respectively. The aggregate velocities and their pressure derivatives are $V_P = 9.75$ km/s, $V_P' = 0.056$ km/s/GPa, and $V_S = 5.72$ km/s, $V_S = 0.012$ km/s/GPa. We find that the elastic anisotropy of wadsleyite is intermediate between the two other Mg_2SiO_4 polymorphs, forsterite, and ringwoodite. The anisotropy is only weakly pressure dependent and decreases with increasing pressure. The azimuthal and polarization anisotropy for S waves 14.5% and 12.8% respectively, is almost pressure independent, while the azimuthal anisotropy for P waves decreases from 12.5% at ambient pressure to 10.5% in the upper part of the transition zone (14–17 GPa). Our calculated O atom charges suggest that O1 is the most likely hydroxyl site and remains so throughout the stability field of wadsleyite.