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A first-principle investigation of antigorite up to 30 GPa: Structural behavior under compression

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Abstract

The structure of antigorite (m = 17) has been studied by density functional theory from 0 to 30 GPa. The fourth-order Birch-Murnaghan equation of state fit of the thermally corrected LDA results yields an equilibrium volume (V_0 = 2853.13 Å^3), bulk modulus (K_0 = 64.6 GPa), and its pressure derivative (K_0' = 6.94) in good agreement with experimental results. Two changes in compression mechanism occur at 6.1 and 20.5 GPa, individuating three pressure ranges: (1) in the low-pressure range, the antigorite wave flattens and the interlayer thickness decreases rapidly; (2) in the intermediate-pressure range, in-plane rotations of tetrahedra (ditrigonalization) and then wave-bending become the dominant compression mechanisms; (3) in the extreme-pressure range, the mechanism of wave-bending becomes prevalent. The first change reveals the origin of softening found experimentally near 6 GPa: the change in compression mechanism occurs after the minimal mismatch between T- and O-sheets is achieved and is accompanied by an apparent symmetry breaking: accidental degeneracies of structural parameters between short and long halfwaves are lifted, including T-sheet thicknesses and Si-O bond lengths. In the extreme-pressure range, Si-O-Si angles decrease below 122°, which may be the origin of amorphization found experimentally at similar pressure.

Keywords: Antigorite, first principles, equation of state, structure