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SPECIAL COLLECTION: BUILDING PLANETS: THE DYNAMICS AND GEOCHEMISTRY OF CORE FORMATION

Equation of state of pyrite to 80 GPa and 2400 K

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Abstract

The high-cosmic abundance of sulfur is not reflected in the terrestrial crust, implying it is either sequestered in the Earth's interior or was volatilized during accretion. As it has widely been suggested that sulfur could be one of the contributing light elements leading to the density deficit of Earth's core, a robust thermal equation of state of iron sulfide is useful for understanding the evolution and properties of Earth's interior. We performed X-ray diffraction measurements on FeS_2 achieving pressures from 15 to 80 GPa and temperatures up to 2400 K using laser-heated diamond-anvil cells. No phase transitions were observed in the pyrite structure over the pressure and temperature ranges investigated. Combining our new *P-V-T* data with previously published room-temperature compression and thermochemical data, we fit a Debye temperature of 624(14) K and determined a Mie-Grüneisen equation of state for pyrite having bulk modulus K_T = 141.2(18) GPa, pressure derivative K'_T = 5.56(24), Grüneisen parameter γ_0 = 1.41, anharmonic coefficient A_2 = 2.53(27) × 10^{-3} J/(K^2·mol), and q = 2.06(27). These findings are compared to previously published equation of state parameters for pyrite from static compression, shock compression, and ab initio studies. This revised equation of state for pyrite is consistent with an outer core density deficit satisfied by 11.4(10) wt% sulfur, yet matching the bulk sound speed of PREM requires an outer core composition of 4.8(19) wt% S. This discrepancy suggests that sulfur alone cannot satisfy both seismological constraints simultaneously and cannot be the only light element within Earth's core, and so the sulfur content needed to satisfy density constraints using our FeS_2 equation of state should be considered an upper bound for sulfur in the Earth's core.

Keywords: High-pressure, diamond-anvil cell, equation of state, X-ray diffraction