

CHEMISTRY AND MINERALOGY OF EARTH'S MANTLE

Raman spectroscopy of siderite at high pressure: Evidence for a sharp spin transition

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ABSTRACT

We have measured high-pressure Raman spectra of both siderite single-crystalline and polycrystalline powder samples in diamond-anvil cell experiments across the pressure-induced high-spin (HS) to low-spin (LS) transition of Fe²⁺. Between 43.3 and 45.5 GPa, we observed a color change from transparent to green, which is associated to the spin transition. Furthermore, we calibrated the position of the Raman active ν_1 mode with pressure. In a second diamond-anvil cell experiment, we observed the color change from transparent to green in the form of a transition front passing through the single crystal and collected Raman spectra across the transition front. We were able to constrain the stress variation across this transition front to about 0.2 GPa, well below the resolution of our Raman-based pressure/stress calibration. In contrast to the single crystal, the powder sample shows the spin transition over a pressure range of 5 GPa, which we attribute to intergranular stresses. We conclude that within the resolution of our stress/pressure calibration the spin transition of iron in single-crystalline siderite is sharp.

Keywords: Siderite, high pressure, carbonates, spin transition