Electronic spin transition in siderite at high pressure studied by Raman spectroscopy: Evidence for a sharp spin transition

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Siderite ($FeCO_3$) is one of the most common carbon bearing minerals on Earth and consequently one of the most likely carbon bearing minerals to be subducted into the deep Earth. Many previous studies already confirmed the stability of siderite up to depths of the lower mantle and observed between 40 and 50 GPa an electronic high spin to low spin transition [1, 2, 3, 4]. But there is a conflict regarding the mechanism of the spin transition since some studies observe with Raman spectroscopy a gradual spin transition over a pressure range and some studies observe with XRD a sudden spin transition. Furthermore the spin transition is accompanied by a color change from transparent (HS) to green (LS). This color change was observed in form of a transition front from HS to LS at 44 to 45 GPa [3].
In order to check how the three observations from XRD, Raman spectroscopy and the color change combine, we measured Raman spectra along a transition front similar to the one previously observed [3] and checked whether this transition front is caused by pressure gradient or whether the spin transition is actually sharp.
Our spectra indicate that there is only a very small pressure gradient. Furthermore, the Raman active v1-mode was calibrated against pressure in order to quantify the pressure gradient. We were able to see that the pressure gradient is only about 0.2 GPa along the transition front and therefore the spin transition might even be instantaneous.

[1] Lavina et al. (2010) *Phys. Rev. B* **82,** 064110. [2] Cerantola et al. (2015) *Am. Min.* **100**, 2670-2681. [3] Lobanov et al. (2015) *Am. Min.* **100**, 1059-1064. [4] Spivak et al. (2014) *Phys. Chem. Minerals* **41**, 633-638.