Electronic origins of the giant volume collapse in the pyrite mineral MnS$_2$ - DTU Orbit

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The pyrite mineral MnS$_2$ was recently shown to undergo a giant pressure-induced volume collapse at $\sim$ 12 GPa, via a disordered intermediate phase. The high pressure arsenopyrite phase is stabilised by metal-metal bonding, a mechanism now shown to be ubiquitous for Mn$^{2+}$ chalcogenides. Here we report a spectroscopic investigation of this transition up to pressures of 22 GPa. Using XANES we show that the transition does not involve a change in oxidation state, consistent with the arsenopyrite crystal structure proposed at high pressure. Notably, the XANES spectrum is almost identical in the pressure-induced disordered phase, and after crystallisation induced by laser-heating. The former is therefore a 'valence bond glass', and is likely disordered due to kinetic hindrance of the phase transition. We also detect electronic changes in the compressed pyrite phase, and this is confirmed by Raman scattering which shows that the disulphide vibrations in the pyrite phase saturate before the volume collapse. Together with detailed DFT calculations, these results indicate that electronic changes precede valence bond formation between the Mn$^{2+}$ cations.

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