Electronic origins of the giant volume collapse in the pyrite mineral MnS2 - DTU Orbit (14/03/2019)

Electronic origins of the giant volume collapse in the pyrite mineral MnS2

The pyrite mineral MnS2 was recently shown to undergo a giant pressure-induced volume collapse at ~ 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 Mn2+ 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 Mn2+ cations.

General information
State: Published
Organisations: Department of Physics, Technical University of Denmark, Neutrons and X-rays for Materials Physics, University of Nevada Las Vegas, University of Bayreuth, Lawrence Livermore National Laboratory, Institut Laue-Langevin, Ehime University, Oak Ridge National Laboratory, European Synchrotron Radiation Facility
Number of pages: 7
Pages: 540-546
Publication date: 2019
Peer-reviewed: Yes

Publication information
Journal: Journal of Solid State Chemistry
Volume: 269
ISSN (Print): 0022-4596
Ratings:
BFI (2019): BFI-level 1
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.2 SJR 0.632 SNIP 0.805
Web of Science (2017): Impact factor 2.179
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.09 SJR 0.618 SNIP 0.871
Web of Science (2016): Impact factor 2.299
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.18 SJR 0.679 SNIP 0.956
Web of Science (2015): Impact factor 2.265
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.35 SJR 0.799 SNIP 1.058
Web of Science (2014): Impact factor 2.133
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.22 SJR 0.769 SNIP 1.036
Web of Science (2013): Impact factor 2.2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.27 SJR 0.931 SNIP 1.184
Web of Science (2012): Impact factor 2.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.5 SJR 1.004 SNIP 1.299
Web of Science (2011): Impact factor 2.159
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.068 SNIP 1.202
Web of Science (2010): Impact factor 2.261
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.057 SNIP 1.325
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.988 SNIP 1.22
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.066 SNIP 1.317
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.033 SNIP 1.319
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.768 SNIP 1.105
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.751 SNIP 1.186
Scopus rating (2003): SJR 0.802 SNIP 1.093
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.871 SNIP 1.234
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.899 SNIP 1.25
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.887 SNIP 1.233
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.951 SNIP 1.234
Original language: English
Keywords: Magnetism, Pressure, Pyrite, Spin-state transition
DOIs: 10.1016/j.jssc.2018.10.032
Source: Scopus
Source-ID: 85055731963
Research output: Research - peer-review; Journal article – Annual report year: 2019