Crystal structures of iron bearing tetrahedrite and tennantite at 25 and 250 degrees C by means of Rietveld refinement of synchrotron data - DTU Orbit (01/12/2018)

Crystal structures of iron bearing tetrahedrite and tennantite at 25 and 250 degrees C by means of Rietveld refinement of synchrotron data

Rietveld refinement of X-ray synchrotron data was performed for two synthetic tetrahedrite samples, with 0.61 and 1.83 Fe atoms, and two synthetic tennantite samples with 0.10 and 1.23 Fe atoms p.f.u. M-12(Sb,As)(4)S-13. Measurements were performed at 25 and 250 degrees C. For both the phases, increased Fe substitution is reflected in the increased tetrahedral 'Cu1'-S distance ('Cu1' is a site of Fe substitution) and Cu2-S distances. Cu2 was refined as a split position; the Cu2-Cu2 split about the plane of the S1(2)S2 triangle is about 0.56 and 0.65 angstrom for tetrahedrite and tennantite, respectively. Cu2-Cu2 distances in the structure cavity are 2.8-2.9 angstrom. Between 25 and 250 degrees C, the lattice parameter a increased by 0.02-0.04 angstrom and the interatomic distances by 0.01 angstrom on an average. Thermal expansion coefficients of little-substituted samples are similar to those of unsubstituted samples, whereas thermal expansion appears to decrease with increasing substitution by Fe. The Cu2-Cu2 split increases at 250 degrees C by about 0.1 angstrom for tetrahedrite and by more than 0.15 angstrom for tennantite but the cage expansion is minimal so that the Cu2-Cu2 distances in the cavity decrease with temperature. Difference Fourier maps indicate that there is little residual electron density left between the two Cu2 half-sites in tetrahedrite but this inter-site density is substantially higher in tennantite. It increases with temperature, especially in the little-substituted tennantite sample.

General information
State: Published
Organisations: Department of Environmental Engineering
Contributors: Friese, K., Grzechnik, A., Makovicky, E., Balic-Zunic, T., Karup-Møller, S.
Pages: 455-465
Publication date: 2008
Peer-reviewed: Yes

Publication information
Journal: Physics and Chemistry of Minerals
Volume: 35
Issue number: 8
ISSN (Print): 0342-1791
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.73 SJR 0.702 SNIP 0.935
Web of Science (2017): Impact factor 1.679
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.39 SJR 0.582 SNIP 0.799
Web of Science (2016): Impact factor 1.521
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 1.33 SJR 0.608 SNIP 0.767
Web of Science (2015): Impact factor 1.585
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 1.59 SJR 0.769 SNIP 0.954
Web of Science (2014): Impact factor 1.538
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 1.46 SJR 0.808 SNIP 0.895
Web of Science (2013): Impact factor 1.403
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 1.33 SJR 0.77 SNIP 0.887
Web of Science (2012): Impact factor 1.304
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 1.71 SJR 1.032 SNIP 1.066
Web of Science (2011): Impact factor 1.73
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.29 SNIP 1.306
Web of Science (2010): Impact factor 1.876
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.015 SNIP 1.1
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.129 SNIP 0.874
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.963 SNIP 0.847
Scopus rating (2006): SJR 1.195 SNIP 1.11
Scopus rating (2005): SJR 0.956 SNIP 1.108
Scopus rating (2004): SJR 1.311 SNIP 1.284
Scopus rating (2003): SJR 1.183 SNIP 1.326
Scopus rating (2002): SJR 1.13 SNIP 0.968
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.675 SNIP 1.18
Scopus rating (2000): SJR 1.247 SNIP 1.354
Scopus rating (1999): SJR 1.236 SNIP 1.081
Original language: English
Keywords: split trigonal planar copper positions, crystal structure at 25 and 250 degrees C, tennantite, iron substitution, Rietveld refinement, tetrahedrite
Source: orbit
Source-ID: 236142
Research output: Research - peer-review ; Journal article – Annual report year: 2008