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

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 distances ('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.

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