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LETTER

Crystal structure of argentopyrite, $AgFe_2S_3$, and its relationship with cubanite

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ABSTRACT

The structure of argentopyrite, $AgFe_2S_3$, was determined for the first time with single-crystal X-ray diffraction. In contrast to the previously reported orthorhombic symmetry, our data show that argentopyrite is monoclinic with space group $P112_1/n$ (non-standard setting) and unit-cell parameters a = 6.6902(2), b = 11.4497(4), c = 6.4525(2) Å, γ = 90.2420(8)°, and V = 494.26(3) Å^3. Similar to cubanite ($CuFe_2S_3$), the structure of argentopyrite is also based on approximately hexagonal close-packed S atoms, with cations ordered over one half of the tetrahedral sites, forming corner-shared AgS_4 and FeS_4 tetrahedral sheets parallel to (001). The two structures differ chiefly in the linkage between the two adjacent tetrahedral sheets and the ordering patterns of cations within a tetrahedral sheet. Topologically, the structure of argentopyrite can be obtained by a displacement of a tetrahedral sheet in the cubanite structure along the ($\boldsymbol{a}$/2 + $\boldsymbol{b}$/6) direction relative to the sheet beneath, giving rise to a cluster of *four* edge-shared FeS_4 tetrahedra in argentopyrite, as compared to *two* in cubanite. There are *two* distinct Fe sites (Fe1 and Fe2) in argentopyrite, rather than only *one*, as in other MFe_2S_3 sulfide minerals (M = monovalent cations). Together with published Mössbauer data, we suggest that there exists some degree of Fe^{2+}-Fe^{3+} order-disorder in argentopyrite, with Fe^{2+} favoring the more distorted Fe2 tetrahedral site. Argentopyrite appears to possess all the features proposed by Putnis (1977) for a high-temperature ordered form of cubanite.

Keywords: Argentopyrite, $AgFe_2S_3$, Ag-Fe sulfides, cubanite-related mineral, sternbergite, crystal structure, single-crystal X-ray diffraction