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The crystal chemistry of Fe-bearing sphalerites: An infrared spectroscopic study

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Abstract

Iron substitution into sphalerite, ZnS, has been studied systematically by infrared spectroscopy. A range of natural and synthetic compositions, $(Zn_{1-x}Fe_x)S$, $0 \le x \le 0.24$, were examined. The IR spectrum of pure ZnS contains a single strong absorption band at 320 cm^{-1}. With addition of FeS, the spectra become broader and shoulders appear. For compositions ≥9 mol% FeS, a splitting of the main peak occurs, and the spectra show two absorption maxima at approximately 300 and 315 cm^{-1}, respectively. The observation of such extra features does not correspond to the usual behavior observed in other ternary mixed crystals, where either one-, two-, or mixed-mode behavior is observed. The spectra can be deconvoluted into up to three peaks, main Peaks A and B at around 300 and 315 cm^{-1}, respectively, and a shoulder at around 330 cm^{-1} (Peak C). The positions and area of the peaks do not change significantly with increasing Fe content. The peak at 315 cm^{-1} is the main absorption peak of the host ZnS structure, and the peak at 300 cm^{-1} is an impurity induced mode. An effective linewidth parameter Δ_{corr} was determined by autocorrelation analysis for each spectrum, but there are no obvious trends in the values of Δ_{corr} that can be interpreted in terms of an inhomogeneous distribution of Fe within the sphalerite structure.

Keywords: Fe-bearing sphalerites, infrared spectroscopy, autocorrelation analysis, solid solution