

IN SITU HIGH TEMPERATURE X-RAY DIFFRACTION CHARACTERIZATION OF SILVER SULFIDE, Ag₂S

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Silver sulfide, Ag₂S is most commonly known as the tarnish that forms on silver surfaces due to exposure of silver to hydrogen sulfide. The mineral acanthite, is a monoclinic crystalline form of Ag₂S that is stable to 176 °C. Upon heating above 176 °C, there is a phase conversion to a body-centered cubic (BCC) form referred to as argentite. Further heating above 586 °C results in conversion of the BCC phase to a face-centered cubic (FCC) phase polymorph. Both high temperature cubic phases are solid silver ion conductors. In-situ high temperature X-ray diffraction was used to better understand the polymorphs of Ag₂S on heating. It was observed that Ag₂S diffracts very weakly, even after annealing at high temperature. In addition, silver whiskers were found to grow from the Ag₂S powder upon annealing.

The existing Powder Diffraction File entries for the high temperature FCC polymorph is of questionable reliability, prompting a full Rietveld structure refinement of the BCC and FCC polymorphs. Rietveld analysis was useful to show that the sulfur atoms are largely disordered and can only be described by unreasonably large isotropic displacement parameters or split site models. We also report the unit cell volume thermal expansion along with the structures.