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The kinetics of the $\alpha \rightarrow \beta$ transition in synthetic nickel monosulfide

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ABSTRACT

The kinetic behavior of the α-$Ni_{1-x}S \rightarrow \beta$-NiS transition was investigated via a series of anneal-quench experiments using Rietveld quantitative phase analysis of powder X-ray diffraction data. Initial compositions of α-$Ni_{1-x}S$ were found to play an important role in the kinetics of the transition. The activation energy (E_a) for this α- to β-phase transition is 16.0 (±0.5) kJ/mol for NiS in the temperature range 343 to 423 K, and 13.0 (±0.5) kJ/mol in the temperature range 523 to 623 K. For $Ni_{0.97}S$, however, E_a decreases from 73.0 (±0.5) to 17.0 (±0.5) kJ/mol over the course of the reaction in the temperature range 573 to 593 K. The relationship between E_a and extent of transition (y) for the initial bulk $Ni_{0.97}S$ was derived using the Refined Avrami method. For Ni-deficient compositions, α-$Ni_{1-x}S$, the transformation to β-NiS is accompanied by the exsolution of a progressively more Ni-deficient α-$Ni_{1-x}S$ and Ni_3S_4, and the reactions become more sluggish for more metal-deficient compositions.

Keywords: XRD data, NiS, crystal synthesis, α-NiS, kinetics, nickel monosulfide