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Thermodynamic and experimental simulation of interactions in the Ta-ZnS system

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Abstract

The article presents the results of studies to estimation the possibility of sulfiding of metallic tantalum by zinc sulfide in an inert atmosphere. To theoretically substantiate the possibility of the process, the HSC 6.12 Chemistry software package (Outotec) was used, which allows predicting the equilibrium composition of the interaction products. The Gibbs energies of possible reactions in the ZnS-Ta system are calculated, the optimum operating parameters of the process of complete transformation of metallic tantalum into TaS_2 are determined. Experimental studies were carried out in a tubular furnace in a flow of an inert gas (helium) supplied through a closed loop of an alundum reactor. Components with different molar ratios compressed into tablets were kept at the temperature 1300 °C for 90 minutes. It has been found tantalum disulfide of two modifications (hexagonal and trigonal systems) and Ta_5S_8 (14.1%) are formed at a stoichiometric ZnS / Ta molar ratio of 2.0. Its subsulfides ($Ta_{1.23}S_2$, $Ta_{3.1}S_6$, TaS (y)), which are intermediate phases in the transformation of tantalum-to-TaS_2, are formed if a sulfidizer is deficient. The identification of the phases and the estimation of their proportion in the sulfiding product were made by the full-profile analysis by Rietveld method. The experimental conditions did not reveal the formation of complex sulfides like the Zn_xTaS_2, the formation of which is possible because of zinc intercalation between the layers of the tantalum disulfide basic structure of the crystal lattice.

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