

Thermodynamic modeling of phase formation during the oxidation of niobium aluminide

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Abstract

The results of thermodynamic modeling of oxidation Nb-Al alloy representing intermetallide – NbAl₃ by minimizing of the thermodynamic potential using the software package Chemistry HSC 5.1 (Outokumpu). Chemical transformations in the systems NbAl₃ – CaO₂, NbAl₃ – NaNO₃ and NbAl₃ – Na₂CO₃, NbAl₃ – CaCO₃ in the temperature range 25-1000 °C have been considered. Thermodynamic modeling results indicate the possibility of complete oxidation NbAl₃ using sodium oxide and calcium compounds in air, thus formed niobates and sodium aluminate (calcium). The most suitable oxidation sublimates activator is sodium carbonate by reacting with oxide NbAl₃ intermetallic compounds of Na and Ca in air. Sodium nitrate has the same properties, but its use requires special precautions. Complex calcium alumino-niobates is formed by the reaction NbAl₃ with CaCO₃ and CaO₂, impeding the separation of niobium and aluminum by leaching.