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THERMODYNAMICS AND CHEMICAL ....

低温水相一步合成钡酸盐: 热力学模型建立及验证研究

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摘要 A thermodynamic model has been developed to determine the reaction conditions favoring low temperature direct synthesis of barium titanate (BaTiO3). The method utilizes standard-state thermodynamic data for solid and aqueous species and a Debye-Hückel coefficients model to represent solution nonideality. The method has been used to generate phase stability diagrams that indicate the ranges of pH and reagent concentrations, for which various species predominate in the system at a given temperature. Also, yield diagrams have been constructed that indicate the concentration, pH and temperature conditions for which different yields of crystalline BaTiO3 can be obtained. The stability and yield diagrams have been used to predict the optimum synthesis conditions (e.g., reagent concentrations, pH and temperature). Subsequently, these predictions have been experimentally verified.As a result, phase-pure perovskite BaTiO3 has been obtained at temperature ranging from 55 to 85℃ using BaCl2,TiCl4 as a source for Ba and Ti. and NaOH as a orestatar.

关键词 钡酸盐 一步合成水相 热模型 热力学分析 相平衡图 预测率

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Low Temperature-One-Step Synthesis of Barium Titanate: Thermodynamic Modeling and Experimental Synthesis

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Abstract A thermodynamic model has been developed to determine the reaction conditions favoring low temperature direct synthesis of barium titanate (BaTiO3). The method utilizes standard-state thermodynamic data for solid and aqueous species and a Debye-Hückel coefficients model to represent solution nonideality. The method has been used to generate phase stability diagrams that indicate the ranges of pH and reagent concentrations, for which various species predominate in the system at a given temperature. Also, yield diagrams have been constructed that indicate the concentration, pH and temperature conditions for which different yields of crystalline BaTiO3 can be obtained. The stability and yield diagrams have been used to predict the optimum synthesis conditions (e.g., reagent concentrations, pH and temperature). Subsequently, these predictions have been experimentally verified.As a result, phase-pure perovskite BaTiO3 has been obtained at temperature ranging from 55 to 85℃ using BaCl2,TiCl4 as a source for Ba and Ti. and NaOH as a orestatar.

Key words nanoparticle synthesis thermodynamic modeling barium titanate precursor phase

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