Preparation of magnesium diniobate by solid-state reactions and its role for hydrogen storage

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ABSTRACT

A ternary compound of magnesium diniobate (MgNb $_2$ O $_6$) was prepared by solid–state reactions in order to understand the role of transition metal oxides as a promoter/catalyst for hydrogen storage in Mg/MgH $_2$ systems. MgNb $_2$ O $_6$ was prepared in almost pure form in oxidizing conditions by annealing a stoichiometric mixture of MgO and Nb $_2$ O $_5$. The effect of calcination temperatures on phase formation, reaction kinetics, and heat of reaction of the solid–state product was investigated by ex situ, in situ X-ray diffraction (XRD), and differential scanning calorimetry (DSC). Hydrogen sorption properties of the compound were investigated by mass spectrometer. The crystallographic parameters of binary and ternary Mg–Nb–O phases were extracted by Rietveld method. During solid–state synthesis, the formation of MgNb $_2$ O $_6$ provides single-step reaction between precursor materials proved by in situ experiment and the heat of formation as well as driving force was calculated from calorimetric analysis.

KEYWORDS

Solid–state synthesis; Magnesium diniobate; X-ray techniques; Reaction kinetics; Rietveld refinement

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