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Review Article

A review on kinetic models and corresponding analysis methods for hydrogen storage materials

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ABSTRACT

Analysis of the hydrogenation and dehydrogenation behaviors by kinetic models is an efficient approach to the in-depth understanding of the kinetic mechanism for hydrogen storage materials. A large number of kinetic models as well as analysis methods based on these models have been extensively applied in hydrogen storage materials, and kinetic parameters with physical interpretations are determined to reveal the kinetic mechanism of hydrogenation and dehydrogenation reactions. However, the assumptions and derivation steps of these models are usually difficult to find, and the selection of analysis methods is sometimes confusing. Moreover, some recently proposed models and analysis methods have not been introduced to investigate the kinetic mechanism of hydrogen storage materials yet. These problems significantly prevent the kinetic models as well as analysis methods from further revealing the kinetic mechanism for hydrogen storage materials. Therefore, this review mainly focuses on the illustration of the assumptions and derivation steps of the kinetic models, summarization of corresponding analysis methods, and introduction of some recently proposed kinetic models and analysis methods for hydrogen storage materials.

Contents

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Introduction

Hydrogen storage is one of the key challenges for the widespread application of hydrogen energy [1]. Hydrogen storage materials (HSM), such as MgH_2, $NaAlH_4$, $LiH/Mg(NH_2)_2$ and $LiBH_4$, attracted a significant amount of attention in the past several decades because they can store hydrogen reversibly under relatively moderate condition [2,3]. Numerous efforts have been devoted to the exploration of high-performance catalysts [4,5], hydride-based composition [6], nanosizing [7,8] and new compound preparation [9,10] towards the superior hydrogen storage thermodynamic properties and kinetic performances. One of the hottest topics involved is the in-depth understanding of the kinetic mechanism to develop practical HSM. The kinetic mechanism contains the complicated, time- and space-related factors, including temperature, hydrogen pressure, catalysis, morphology, defect as well as thermodynamic driving force [11].

Analysis of the hydrogenation and dehydrogenation behaviors by kinetic models is an efficient approach to reveal the kinetic mechanisms of HSM [12]. A large number of kinetic models (such as Jander model [13], Ginstling-Brounshtein [14] and Johnson-Mehl-Avrami-Kolmogorov model [15–19]) and corresponding analysis methods (such as Sharp & Jones method [20,21] and Kissinger method [22]) have been extensively applied in the research of HSM. Kinetic parameters with physical interpretations (such as rate constant, activation energy and Avrami exponent) are determined to investigate the hydrogen absorption and desorption kinetic behaviors [7,23,24].

However, there still exist some problems that prevent the kinetic models from accurately describing the absorption and desorption behaviors of HSM. First, it is sometimes difficult to find the detailed assumptions and derivation steps of the kinetic models, which usually leads to the misunderstanding of kinetic mechanism. Second, though numerous analysis methods based on the kinetic models for HSM have been proposed, it is difficult for the researchers to select the proper methods to analyze the experimental data. Last but not least, several more recently developed kinetic models and analysis methods have not been introduced in HSM yet, which may be superior to the present applied models and methods, as higher accuracy and/or more kinetic information can be obtained.

This review mainly focuses on three aspects: (1) illustrate the assumptions and derivation steps of the kinetic models for HSM in detail; (2) systematically summarize the analysis methods on the basis of the kinetic models; (3) introduce new models and corresponding analysis methods that can be potentially applied in HSM.

General principles

Hydrogen can be stored in HSM through physical bond (such as metal-organic frameworks (MOFs), clathrates and carbon nanomaterials) and chemical bond (such as metal hydrides, complex hydrides and metal amides). It is found that most of the kinetic investigations focus on HSM that store hydrogen by chemical absorption and desorption. Therefore, in this work, we mainly review the kinetic models and corresponding analysis methods for HSM that store hydrogen through chemical reaction. The nature of the hydrogenation and dehydrogenation processes of HSM are solid-state reactions, especially gas–solid reactions [25]. So the kinetic models for HSM are mainly on the basis of (but not totally the same to) the models of solid-state reactions [26–29].

Geometrical contraction and nucleation-growth-impingement are two possible reaction modes for hydrogen absorption and desorption, which have been confirmed by theoretical and experimental investigations [23,30]. So the kinetic models for HSM can be divided into two categories according to the reaction modes (see Table 1), which are presented in details in Section Kinetic models. It should be noted that some new models which have not been applied in HSM are also presented in this review, since these models may be superior to the existing models under some certain conditions.

On the basis of the kinetic models, analysis methods like isothermal fitting methods and non-isothermal calculating methods are proposed for HSM. In addition, an isothermal and non-isothermal simultaneously fitting method is recently proposed, which can extract more kinetic information from