KINETIC ANALYSIS OF THE THERMALLY INDUCED TRANSFORMATIONS OF CALCIUM HYDROXIDE IN DIFFERENT GASEOUS ATMOSPHERES

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Keywords: calcium hydroxide, thermal decomposition, solid-gas reaction, impact of water vapor, kinetics

The atmospheric gas that contributes to the thermally induced reaction in the solid–gas system as the product or reactant is one of the most relevant factors to control the kinetics and mechanisms of the reaction. Because of the heterogeneous feature of the reactions in the solid–gas system, change in the atmospheric conditions imposes the dramatical change in the physico-geometrical reaction mechanism and overall kinetics in a complex manner of the interactions of the component physico-chemical reaction steps.

Thermally induced transformations of $Ca(OH)_2$ are such examples. The thermal decomposition of $Ca(OH)_2$ in flowing dry N_2 gas proceeds via partially overlapping two reaction steps attributed to surface and interfacial reactions [1]. The kinetic feature is described by the cumulative kinetic equation [2].

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \sum_{i=1}^{N} c_i A_i \exp\left(-\frac{E_{\mathrm{a},i}}{RT}\right) f_i(\alpha_i) \tag{1}$$

where c_i is the contribution of the reaction step i.

On heating $Ca(OH)_2$ in flowing N_2 – CO_2 mixed gas, masschange curve exhibits a smooth mass gain, which is invariant irrespective of CO_2 concentration (Figure 1(a)). The reaction is interpreted as the consecutive process of the thermal decomposition of $Ca(OH)_2$ and subsequent carbonation of CaO to form $CaCO_3$. The overlapping mass-loss and massgain processes that do not appear on the experimentally resolved mass-change curve can be simulated by the kinetic deconvolution analysis based on eq. (1) [1].

The thermal decomposition of $Ca(OH)_2$ is a typical reversible process in solid–gas system. Therefore, the water vapor pressure $p(H_2O)$ in reaction atmosphere restrains the reaction rate, indicating systematic shift of the mass-loss curve recorded under nonisothermal conditions at a selected heating rate to higher temperatures with increasing $p(H_2O)$ (Figure 1(b)). The kinetics of the reaction over different $p(H_2O)$ is universally described by introducing an appropriate accommodation function in the fundamental kinetic equation.

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = A \exp\left(-\frac{E_{\mathrm{a}}}{RT}\right) f(\alpha) a(p(H_{2}O), P_{\mathrm{eq}}(T))$$
(2)

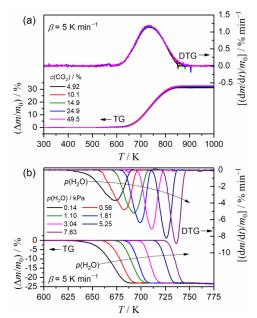


Figure 1. TG–DTG curves for Ca(OH)₂ recorded under different atmospheric conditions in flowing (a) N₂–CO₂ and (b) N₂–H₂O mixed gases.

The practical kinetic analyses for those complex reaction processes are demonstrated in this presentation.

Acknowledgments

The present work was supported by JSPS KAKENHI Grant Numbers 17H00820.

References

- 1. Koga N, Kodani S. Thermally induced carbonation of $Ca(OH)_2$ in a CO_2 atmosphere. PCCP. 2018, 20:26173-26189.
- 2. Koga N, et al. Multistep thermal decomposition of granular sodium perborate tetrahydrate. PCCP. 2018, 20:12557-12573.

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