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Numerical simulation of yttrium oxide grain sintering

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Yttrium oxide is a promising and poorly studied material for the field of catalysis. It can be used as a support in catalytic processes such as carbon dioxide reforming of methane and CO_2 methanation. Predicting changes in the texture of Y_2O_3 during temperature treatment is an important material science and a computational task.

In this study, we applied a phase-field approach to obtain an accurate mathematical description of Y_2O_3 sintering over a wide temperature range. The general principle of the phase-field method is to describe physical quantities by a set of continuous fields that take constant values in specific regions and smoothly change in the interfaces between these regions. In the case of sintering, such areas are the individual grains of the material. The interface of the microstructure has a finite width along which the sintering materials move. The Allen-Cahn and Cahn-Hilliard equation system is used to describe changes in order parameters and mass density distribution.

To verify the mathematical model, yttrium oxide sintering experiments were carried out and data on the textural and structural properties of Y_2O_3 were obtained. The developed model makes it possible to calculate the decrease in the specific surface area and pore volume of yttrium oxide for pores ranging from 3 to 70 nm and determine the growth rate of Y_2O_3 crystallites during sintering. The model allowed us to determine that stepwise heating from 600° C to 900° C and then 1200° C decreases the specific surface area of yttrium oxide from 54 m^2/g to 15 m^2/g and then to 5 m^2/g, respectively.

It should be noted that the obtained experimental micrographs of the cross sections of yttrium oxide samples are in visual accordance with the model images. The approach used in work can be used to predict the evolution of the textural properties of porous materials (catalysts, sorbents, ceramics) under high-temperature conditions.

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