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Possibilities of the Quantitative Comparison of Catalytic Capacity in Autocatalytic Processes of Palladium-Containing Nanocatalysts

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ABSTRACT

When studying the nanocrystalline state, in some cases, an increase in functional activity is observed with an increase in the size of nanoparticles. In this case, the most active atoms are situated on the faces and have a higher coordination in comparison with the atoms on the tops and the edges. One of the explanations for this phenomenon is the formation of hypercycles due to the occurrence of autocatalytic processes. For oscillatory processes inherent in autocatalysis, when the parameters of a nonequilibrium process change over time, it is difficult to apply traditional methods of processing the results of analytical studies. In this regard, it is necessary to develop a methodology for a comparative study of short-term parameters of processes on the same scale, highlighting the main ones and eliminating insignificant and random ones, such as the phase shift at the beginning of self-oscillations or time-localized deviations from activity. This paper presents the results of such a study on the example of palladium-containing nanosystems in the reaction of low-temperature oxidation of CO. It is shown that the study of the behavior of nanocatalysts during the formation of hypercycles is informative using the calculated generalized parameters of the process

KEYWORDS

Carbon Fiber Materials, Carbon Monoxide, Catalysts, Mathematical Modeling, Nanocrystalline, Nanoparticle Size, Nanosystems, Oxidation, Palladium, Size Effect

INTRODUCTION

The high activity of nanoparticles is explained by electron and geometric effects, although this division is very conventional because both effects have the same source, that is, a small particle size (Kempkes et al., 2019, Anwar et al, 2019, Zhizhin 2019). Obviously, there is also a lower activity limit, usually exceeding approximately the cluster size, i.e. a region of optimal size is always observed,

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within which the activity of nanoparticles is maximum. The relationship between size and activity is the most intriguing area of nanosystem science (Casañola-Martin, 2019). Of particular interest is the question of the upper boundary of particle sizes. It is believed that the main scope of investigations in this area is to determine the critical particle size, below which the characteristic properties of nanocrystals become observable, and above which the material behaves like a bulk material (Gusev et al., 2004, Rasulev et al, 2012). The previously proposed method for determining the boundary dimensions, based on serial experiments and the use of methods of mathematical statistics – "model of balls coloring" (Rakhimov et al., 2019) made it possible to determine that in some cases the upper limit is significant - from 100 nm to half a micron . In particular, this phenomenon is observed in the study of the oxidation of carbon monoxide with oxygen.

Since the geometric effect of catalysis depends on the ratios of the number of atoms distributed on the faces, on the edges and tops of the nanoparticle, we can say that in these cases the atoms on the faces with a higher coordination are more active than the atoms on the vertices and edges. Therefore, the rate of the catalysed reaction will be increased by the larger particles. It is shown theoretically that in this case the behavior of ensembles with the formation of hypercycles is possible, when oxidation is realized by waves of self-oscillations (Kalgin, 2011). However, these phenomena have not been sufficiently studied experimentally. It can be assumed that the main obstacles in this are methodological in nature. In this paper, we attempted to use the measurement of "instantaneous" values of catalytic activity to hypercycles' study.

RESULTS AND DISCUSSIONS

The study of the catalytic properties of palladium-containing nanocatalysts in the reaction of low-temperature CO oxidation showed a clear presence of oscillations (Figure 1), when catalytically active structures are formed after exposure to the substrate for a certain time, i.e., a phenomenon called "training" of the catalyst is observed (Bol'shakov et al., 2001). Since according to J. Von Neumann (Von&Burks 1996) the ability to reproduce itself depends fundamentally on the complexity of the organization, and there is a well-defined critical level of complexity, starting from which it becomes self-sustaining or even can grow (Kureychik et al., 2007). In this case, the ability to train indicates a high probability of the formation of catalytic hypercycles (Gorovoy 2018) i.e., systems in which autocatalytic (i.e., self-reproducing) units are, in turn, interconnected through cyclic communication. Scientific interest in such processes is constantly growing, starting with the works of Prigogine, but despite this, there are practically no studies on the study of hypercycle structures for specific autocatalytic reactions.

It is reasonable to assume that one of the stumbling blocks is the lack of a developed methodology for the comparative study of "instantaneous" characteristics of autocatalytic processes, in particular, for processing measurement results (Mukhamediev et al., 2015).

Autocatalysis during oxidation with oxygen is not always manifested, and this depends on the nature of the catalyst carrier, its structure and heterogeneity. Thus, autocatalysis is observed in some cases with the use of some crystalline carriers-chromium oxide, alumochrome, as well as some polymer fibers (activated carbon fibers), but in most cases there is a reduction of palladium ions to metal with the oxidation of CO to dioxide (Rakhimov et al., 2014). The method of application of the active component, the state and availability of surface-active nanoparticles, the location of active centers (for example, on the faces or edges of nanocrystals); the presence of inhibitors and promoters, including those formed or desorbed from the carrier; temperature, pressure, flow rate and its laminarity/turbulence, etc. are also important.

A number of factors have a random character, which is not related to the measurement error, but is fundamentally unavoidable, due to the nature of the functionality of the nanostructures themselves.

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