


Calculation of the Boundary Dimensions of Functionally Active Nanoparticles

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ABSTRACT

Size is a key characteristic of nanoparticles that determines whether the objects belong to this category. Currently, there are not enough experiments on materials of the same chemical composition but of different dispersion in particle size, with equal size of the particles or grains of each sample of material investigated. In the present article, the authors show that the effect of the dispersion of the particle size determines whether the size dependence of a specific property can be calculated alternatively to the direct measurements. By finding the correlations between nano-properties and content of nanoparticles' fractions of different sizes, the boundary conditions can be calculated.

KEYWORDS

Air Purification, Carbon Monoxide, Life Support, Mathematical Modeling, Nanocatalysts, Nanoparticles, Palladium

INTRODUCTION

It became quite obvious that not only the composition, but also the size of nanoparticles can have a key effect on their properties (Gajewicz et al, 2015, Rasulev et al, 2012), in particular, on the catalytic activity. Catalytic processes depend on the coordination of atoms. The atoms located on the faces have a higher coordination than the atoms on the vertices and edges (Ni & Wang 2015). If atoms in low coordination are the most catalytically active, the catalytic activity increases with decreasing particle size. In another case, if the atoms located on the faces are catalytically active, the rate of the catalyzed reaction will be increased by larger particles.

This approach provides an understandable qualitative explanation, but does not allow quantitative determination of the particle size boundaries in which the catalytic effect persists (Wang & Lu 2020). In the available open-access literature, it was not possible to find methods for calculating the position of these boundaries, although approaches to quantitatively predicting the size of particles during their formation are being successfully developed (Handwerk et al., 2020).

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Classic monograph on Nanotechnology (Gusev & Rempel 2004) emphasizes: “The main scope of investigations of the nanocrystalline state is answering the following questions: “Is there a sharp, distinctive boundary between the bulk and the nanocrystalline states? Is there some critical grain (particle) size at which the characteristic properties of nanocrystals become observable, and above which the material behaves as a bulk one?” In addition – not only below, but also above. This main scope may be decided by using the mathematic modelling approaches.

This investigation is an attempt to find in first approximation approach the solution to this important question. The best example for application of this approach can be the case when nano-property is observed on medium size particles. One of such system is present in nano-sized catalysts. It is known that if the atoms located on the faces are catalytically active, the rate of the catalyzed reaction will be increased by larger surfaces of particles (Goodman 1994).

OBJECTS OF EXPERIMENT

As the quantitative statistical characteristics reflecting the average relative values of the active surface of nanomaterials are prompted to introduce the rms diameter and polydispersity index of nanoparticles (Rakhimov 2014). The question is: from which size dimension of particles some special properties getting acquired, namely are there nano-structure properties appearing, and at what size dimensions are they appearing? What can be considered as a nanoparticle with all their acquired features?

Special drawing catalysts comprising platinum metals, palladium and platinum, as active ingredients, were investigated, Table 1. Fiber polymers - polypropylene fiber, polyacrylonitrile, carbon fibers, low modulus carbon, fibrous materials obtained by carbonization and subsequent activation of mats from “Mtilon-M”, copolymers of polyacrylonitrile and hydrocellulose, were used as bearers.

The possibility of exhaustive removal of toxic components, mainly CO, from air by passive systems has been achieved with advent of nanocatalysts (Rakhimov et al., 2014). A decisive influence of substrates nature on the activity and stability and the process character was determined (Rakhimov et al., 2014; Nurmukhammadov et al., 2014; Smanova et al., 2011; Madusmanova et al., 2020). At the same time, it is obvious that the state and also physical and chemical characteristics of active component will exert not smaller influence on properties of the catalytic system in whole.

Activity of catalysts was determined by decreasing the CO content in gas-air mixture at room temperature. The rms diameter and coefficient of polydispersity of nanoparticles (Rakhimov 2014) were measured by transmission electron microscopy, Table 1.

RESULTS AND DISCUSSION

Catalytic Activity as A Special Nanoparticles Property

For investigation of the influence of qualitative changing of nano-composites properties the most evident observations of peculiar properties related specifically to nano-particles can be used. As such peculiar properties can be attributed to effect shown by drawing palladium nano-catalysts at low-temperature oxidation of CO by oxygen. The exhaustive removal of CO by oxygen’s catalytic oxidation in air at room temperature in real experiments do not usually traced neither for too small (solutions, solid solutions) nor for too large (large particles) objects of similar chemical compositions (Rakhimov et al., 2014).

Are There Any Exclusive Properties of Nanoparticles?

Before construction of the model, it is necessary to state the following: there are present or not present some qualitative, spasmodic changes in properties inherited to substances characterized specifically by nano-sized dimensions. If such changes are absent, then only quantitative inter-relationship of

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