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PHENOMENOLOGICAL THERMODYNAMICS OF ADSORPTION FOR JUSTIFICATION OF SYNTHESIS OF THE OPTIMAL HYDROGEN ACCUMULATOR BASED ON ZEOLITES, CARBON NANOTUBES AND NANOSPHERES

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1. INTRODUCTION

The progress in the use of hydrogen as ecologically pure fuel depends upon solution of the problem of safe and cheap method for its storage. The organization of the optimal sorption process, the adsorbent synthesis with the necessary selectivity in respect to hydrogen as well as the elucidation of a mechanism of the adsorption and catalytic process require a theoretical description.

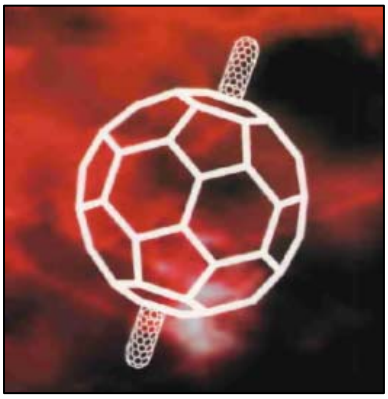

Figure 1. Carmon nanomateriaks

The purpose of the work is to provide a phenomenological thermodynamic description of the sorption process and carry out a search for an analytical solution providing the creation of a material being capable to retain hydrogen for a long time with a big volumetric filling.

The adsorption process description at the molecular level has been developed over two parallel directions, namely: the first direction comprises works by Gibbs who created the thermodynamic theory of adsorption; the second direction comprises works by Polyany who created the potential theory of adsorption describing physical adsorption. It is well-known that the diffusion coefficients and the diffusion process activation energy depend upon the ratio between the hydrogen molecule diameter (d=0.289nm) and the inlet pore diameter (M.M. Dubinin, D.P. Timofeyev) [1,2].

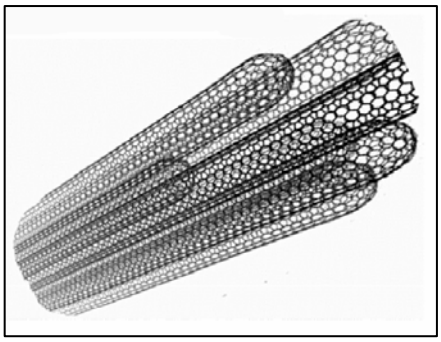

Figure 2. Carbon nanotube

The adsorbent structure and properties strongly influence on its main characteristics, i.e. adsorption capacity, adsorption rate, etc. According to the M.M. Dubinin's classification, all kinds of adsorbents are divided into the following structural groups [2]:

- adsorbents with micropores, which sizes are comparable with the molecule diameters. In such pores, the adsorption potentials grow due to fact that the fields of adsorption forces being created by the pore walls are overlapping, the differential adsorption heat increases and the adsorption value rises,
- adsorbents with big pores where no adsorption potential rise is present,
- adsorbents with transition pores.

2. METHODS

By means of an analytical method and with the use of a phenomenological thermodynamic description of the process, a conclusion has been made on a possibility of hydrogen accumulation in the adsorbent pores and its long-term retaining under technically acceptable ambient parameters.

3. APPROACHES

If the adsorbent pores by their dimensions are comparable with adsorbate molecules, the adsorption process acquires an activated nature. In this case, essential becomes the presence of a potential barrier at the pore inlet. The availability of a potential barrier, on the one hand, complicated the microsorbent filling process and, on the other hand, is a retaining factor decelerating the desorption.

4. NOVELTIES

A phenomenological thermodynamic description has been created for the process of sorption of the adsorbents in question. A scientifically justified model of the optimal hydrogen accumulator and the its filling conditions have been obtained. It has been proposed to create the optimal hydrogen accumulator, to perform synthesis of a special adsorbent with the capillaries being equal or less by their diameters than the hydrogen molecule. In order to implement the filling process, the following technology has been proposed.

The adsorbent is to be placed in a process chamber and vacuumed up to 10^{-3} – 10^{-5} Pa; pure hydrogen (hydrogen purity is 99.999%) heated up to 300°C is to be fed into the chamber until the atmospheric pressure is established in the process chamber. Then a four-hour adsorbent holding in the hydrogen atmosphere shall be carried out. After that, the temperature shall be reduced and the pressure shall be released from the chamber.

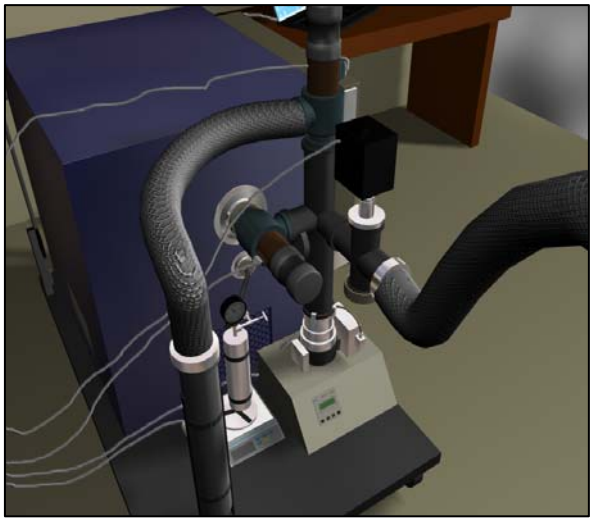

Figure 3. The stand of saturation

5. RESULTS

The analysis of bibliographic data proves the objectiveness of approach proposed.

6. CONCLUSION

At the present time, the existing technologies on growing zeolites, carbon nanotubes and nanospheres with the given pore sizes can provide the fulfillment of the approach proposed. The creation of a sorption substance with a high potential barrier provides a long-term hydrogen retention in the hydrogen accumulator with the operational temperature being acceptable

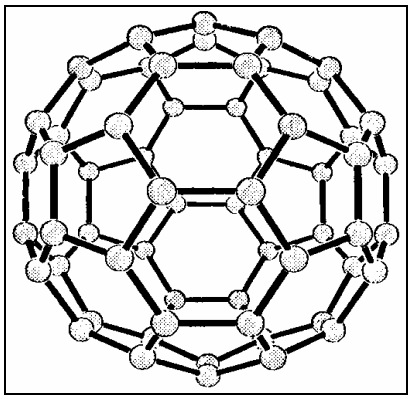

Figure 4. Molecule C_{60}

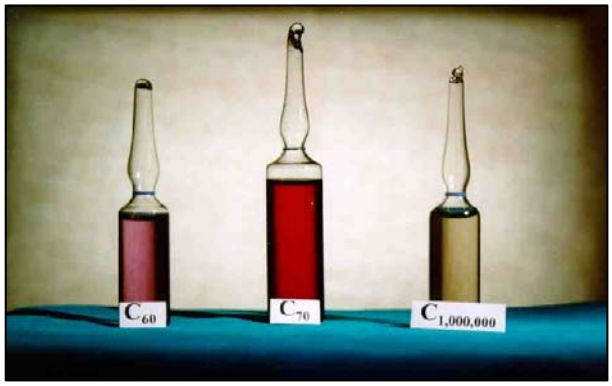

Figure5. The molecules C_{60} , $C_{70,}$ $C_{1,000,000}$ dissolved of toluene

ACKNOWLEDGEMENTS

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[1]. D.P. Timofeev. – "Adsorption kinetics", - USSR Academy of Sciences Publishers. M. 1962.

[2]. M.M. Dubinin, V.V. Serpinsky. – "Adsorption in micropores". – Proceedings of the 5th Conference on adsorption theory". - USSR Academy of Sciences. "Nauka" Publishers. M. 1963.