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Mechanisms of Hydrogen Sorption, Solubility and Diffusivity in Carbon Nanomaterials, Relevance to the On-Board Storage Problem

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1. Introduction

Thermodynamic analysis [1,2] of the most significant experimental data on the hydrogen sorption by graphites and related novel carbon-based nanomaterials at room temperatures and technological pressures (fullerenes, single- and multi-wall nanotubes, nanofibers, nanostructured graphites) is performed.

The thermodynamic and kinetic (diffusion) characteristics of sorption processes are refined and compared with the theoretical quantities, for optimizing and a better understanding of the interaction between hydrogen and carbon materials.

The attention is concentrated on the unique Rodriguez-Baker studies [3] of graphite nanofibers (charged at hydrogen pressure of 11 MPa), where a super hydrogen adsorption capacity (H/C ≈ 6-8) has been found.

2. Discussion - analytical results

As our analysis has shown [1,2], a considerable part of the anomalous data [3] (~30 % of the total storage amount) is in a satisfactory accordance with most of other known data, particularly, with the data [4] of S. Orimo et al. on mechanical synthesis of hydrogen with graphite (charged at 1 MPa) and the recent data [5] of I.O. Bashkin et al. on graphite nanofibers and single-wall nanotubes (charged at 9 GPa)). As is also shown [1,2], the hydrogen bulk and "grain boundary" concentrations in specimens [3] (after a fast release from them of ~70 % of adsorbed hydrogen) are about of a "carbohydride" value (H/C ~ 1). A similar situation is in specimens [4,5].

The extreme anomalous part (~70 %) of the adsorbed hydrogen in specimens [3] might be related to an unknown physical-chemical mechanism of adsorption. It is consistent with the neutron diffraction data of M. Nielsen et al. about a high-density packing of hydrogen adsorbed on graphite (higher than in solid molecular hydrogen) and X-ray data [5] on an anomalous increase (~40 %) of the graphene inter-layer distance.

The energy characteristics of both the chemical and physical interaction of hydrogen with carbon nanostructures are also discussed, particularly, in connection with the analysis [2] of the related data of B.K. Pradhan et al. (Phys. Rev. Lett. (2002)) and the recent review of A.V. Eletskii (Physics-Uspekhi, RAN, Vol. 47, # 11 (2004)).

The characteristics and micromechanisms of hydrogen diffusion in graphites and carbon nanostructures related to the chemisorption and physical sorption processes are considered, particularly, with inclusion of recent diffusion data [6].

3. Conlusion

In many scientific and technological cases, the hydrogen sorption processes in carbon nanomaterials are rate-limited by the hydrogen diffusion transport with fundamental characteristics and micromechanisms, which are rather weakly studied.

There is a real possibility (whith respect to both the experimental and theoretical basis) of developing a super hydrogen carbonaceous adsorbent – a porous carbon-based nanomaterial for the hydrogen on-board storage in fuel-cell-powered vehicles.

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