UDC 620.3
Lushchin S.P.
PhD, associate prof. National University «Zaporizhzhia Polytechnic»

CARBON NANOMATERIAL AS A METHOD OF HYDROGEN STORAGE

The use of hydrogen as an environmentally friendly source of energy largely depends on solving the problem of its storage and transportation. Today the most promising is the use of nanomaterials for hydrogen storage. The hydrogen sorption capabilities of nanomaterials are many times higher than the known methods of hydrogen storage. For this, carbon nanotubes can be used.

Gas storage using carbon nanotubes has attracted a lot of attention after the experiment described in the work of Dillon [1], reporting on the filling of single-walled carbon nanotubes with a diameter of about 1.2 nm with hydrogen.

The value of the specific surface area of carbon nanotubes is about 110 m^2g^{-1}. Experiments show that the specific amount of absorbed hydrogen is tens of times higher than the value that corresponds to the surface adsorption of hydrogen, taking into account the measured value of the specific surface of the nanotube. This fact confirms that the bulk filling of carbon nanotubes with molecular hydrogen is predominant [2].

Let us estimate the possibility of bulk filling of a single-walled carbon nanotube (SWCNT) with molecular hydrogen. The mass density of such a structure in g/mm^3 is determined by the ratio [2]:

$$\rho = \frac{4\sigma_c}{D}, \tag{1}$$

where D – nanotube diameter, 10^{-8} sm; σ_c=0.77·10^{-7} g/sm^2 – maximum surface density of carbon.

The maximum degree of filling SWCNTs with molecular hydrogen is determined by the ratio [2]:

$$\eta_H = \frac{\rho_H}{\rho_H + \rho_C} = \frac{0{,}07}{0{,}07 + 30{,}4 / D}, \tag{2}$$

where ρ_H = 0.07 g/mm^3 – density of hydrogen.

It can be seen from this expression that the degree of filling of SWCNTs increases with an increase in their diameter. The calculation shows that for the degree of filling η_H=6.5 wt.%, which is necessary for using SWCNTs for storing hydrogen, the nanotube diameter should be more than 3 nm. For multilayer nanotubes in the form of a bundle, the sorption capacity η_H = 6.5 wt.% is achieved at a nanotube diameter of 2.1 nm.

Hydrogen penetration into the nanotube cavity can also be activated by the edge modification of the open end using various functional groups, for example, O, OH, and NH_2 [3]. One of the ways to create surface-modified nanotubes is to saturate the outer surface of nanotubes with atomic hydrogen. The mechanism of adsorption of hydrogen atoms on the outer surface of semiconducting single-walled carbon nanotubes is described in detail in [4]. The process of attachment of atomic hydrogen to the surface of single-layer carbon tubulene (*n*, *n*) and (*n*, 0) types is considered. During adsorption the electron density is transferred from the H atom to the surface with the formation of the H+ proton. This proton can migrate over the SWCNT surface.

In our opinion, the use of atomic hydrogen during saturation of nanotubes can increase the degree of penetration of atoms into the nanotube cavity and increase their sorption capacity. This is due to the greater penetrating power of atomic hydrogen. As a result of recombination, atomic hydrogen can be in a molecular state in the cavity of a nanotube, which is a favourable condition for its release during operation.

REFERENCES

1. Storage of hydrogen in single-walled carbon nanotubes / A.C. Dillon, K.M. Jones, T.A. Bekkedahl [et al.] // Nature. – 1997. – Vol. 386. – P. 377.

2. Елецкий, А.В. Сорбционные свойства углеродных наноструктур / А.В. Елецкий // УФН. – 2004. – Т. 70. – С. 1191–1231.

3. Запороцкова, И.В. Исследование влияния краевой функционализации на процессы капиллярного заполнения углеродных нанотрубок водородом / И.В. Запороцкова, Е.В. Прокофьева // Физика волновых процессов и радиотехнические системы. – 2009. – Т. 12, № 4. – С. 107–111.

4. Запороцкова, И. В. Механизмы заполнения однослойных углеродных нанотрубок атомарным водородом / И.В. Запороцкова, Н.Г. Лебедев // Химическая физика. – 2006. – Т. 25, № 5. – С. 91 – 96.