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Abstract

Investigations of Hydrogen Permeability of Nickel Capillaries †

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1. Introduction

One of the global problems of our time is ecology; environmental pollution caused by the growing number of emissions from the combustion of hydrocarbon fuels, including vehicles with an internal combustion engine, which is growing every year. One of the promising directions in this regard is the transfer of transport to hydrogen-oxygen fuel cells, which effectively convert the chemical energy of hydrogen into electrical energy, releasing only water vapor into the atmosphere. At present, fuel cells with a proton exchange membrane (Proton Exchange Membrane fuel cell, PEMFC) are the most promising for transport. However, their application requires the use of ultrapure hydrogen, since even small amounts of CO (at the level of several ppm) in hydrogen, usually obtained by reforming hydrocarbons, poison the electrocatalysts and reduce the efficiency of the fuel cell. The solution to this problem can be the production of ultrapure hydrogen using hydrogen-selective membranes.

This work is devoted to the study of the transport characteristics of nickel hydrogen-selective membranes (nickel industrial capillaries of various thicknesses). In this work, the hydrogen permeability of nickel capillaries of various thicknesses was measured; studies of the mechanism of hydrogen transport through nickel capillaries were carried out using computer simulation.

2. Experimental

Commercially available nickel capillaries were supplied by PJSC "Revda non-ferrous metal processing works" (Revda, Russia). The crystal structure of nickel capillaries before and after hydrogen permeability measurements was examined by X-ray powder diffraction. The XRD experiments were performed using Bruker D8 Advance diffractometer with a high-speed Lynx Eye detector (CuKα radiation). Data sets were recorded in a step-scan mode in the 2θ range of 10–80 with intervals of 0.02°. The qualitative phase analysis was performed using the ICDD PDF-4+ database (2011).

A one-dimensional mathematical model describing the transport of hydrogen through a nickel capillary is based on assumptions similar to those used in [1], namely:

The nickel capillary operates under steady state isothermal conditions.

Diffusion of hydrogen in gas flows is not a limiting stage. The radial inhomogeneity of the composition in gases is insignificant.

The partial pressures of hydrogen on the outer and inner surfaces of the capillary are the same as in the gas phase.

It is assumed that the case in a plug-flow reactor is considered.

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The ideal gas law applies to gas mixtures.

The total pressure in gases is maintained at atmospheric pressure.

It was assumed that the nickel capillary operates under stationary conditions; the partial pressures of hydrogen $pH_{2.1}(x)$ outside and $pH_{2.2}(x)$ inside the capillary depend on the distance x from the entrance to the capillary. The $pH_{2.2}$ value at the outlet of the nickel capillary is determined by the total hydrogen flux passing through the capillary, as well as the sum of the contributions of all local fluxes $F(H_2)$ (x, x+dx) (mol/s) passing through small areas of the capillary surface dS between x and x+dx.

3. Result and Discussion

In this work, the parameter $\gamma(T)$ and E^{eff} of the process of hydrogen transport of nickel capillaries were determined using computer simulation. The calculated values of the parameters $\beta(T)$ are presented in the Arrhenius coordinates in Figure and Table 1.

Table 1. Basic Parameters of the nickel capillaries.

Nickel capillary	Activation energy for hydrogen permeability, Ea /kJ/mol	Pre-exponential factor for hydrogen permeability, $\beta / 10^{-7}$ mol/m/s/Pa$^{1/2}$
L=147 μm	58.34	3.65
L=127 μm	57.49	3.96
L=107 μm	55.95	2.74
L=84 μm	55.58	2.66

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