Simulation of Hydrogen Isotopes Accumulation Processes in Materials in the Presence of Chemical Traps

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The accumulation of hydrogen inside solids occurs in traps of a different nature. In addition to presence of hydrogen in interstitial sites, there are dislocation mechanisms of hydrogen storage, micropores and microcracks, sorption on the free surface of microdefects, chemical traps with the formation of hydrides and other compounds, both with matrix material and with impurities or components of alloys.

It is established that each type of trap has its own hydrogen binding energy, which can vary from 0.2 eV for hydrogen gas in microdefects to several eV for hydrogen chemically bound in traps. Measurements of concentration distribution of hydrogen dissolved in solids over binding energies provide a clue as to the understanding of hydrogen impact on mechanical properties and to the development of technologies for controlling the materials properties during their production and operation.

Therefore, the actual problem is the creation of models that would allow estimating the parameters of traps for hydrogen, based on the data of sorption experiments.

The paper presents the simulation results of experiments on hydrogen saturation of materials in the presence of chemical traps. The proposed model, based on the numerical solution of the diffusion equation in the presence of irreversible capture, made it possible to describe the absorption process and determine the activation energies of hydrogen interaction with the materials.

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Sulfur Polymer as Substrate for Carbon-dot based Counter electrode.

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Dye sensitized solar cells (DSSCs) are efficient and low-cost photovoltaic converters of energy based on the natural dye. The most crucial part of DSSCs is a counter electrode, which is usually coated with an expensive Pt metal or thermally unstable carbon dots. To functionalize this electrode with a cost-effective and easily absorbable material, we used mixed carbon dots with various additives to overcome the challenges of the application process to FTO glass. We showed that using a sulfur-limonene polymer as an additive, the coating can be done at a low temperature with a high absorbance on the electrode.