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Metal Hydride Technologies for Separation of Hydrogen Isotopes

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Abstract. The paper considers the issue of theoretical prediction of characteristics at which separation of hydrogen isotopes occurs in the “gas-metal” system.

Mathematical modeling of sorption is based on the use of the lattice gas model often used for metal hydrides. In contrast to the Leicher ideal solution model, it is taken into account that the dissolution of hydrogen in the metal increases the volume of the crystal lattice. This leads to additional contributions to potential energy. The model also takes into account the interaction between the atoms of the incorporated (absorbed) hydrogen isotopes. These phenomena are described by the methods of thermodynamic perturbation theory.

The different composition of the gas (protium and deuterium) in contact with the metal leads to the fact that sorption, accompanied by the formation of hydride, proceeds for the same temperature at different equilibrium pressures. This phenomenon characterizes the isotope effect. The temperature dependences of the pressure on the "plateau" for palladium hydride and deuteride are obtained. The differences in these pressures can be used for the practical use of metal hydrides in the separation of hydrogen isotopes.

Introduction

The ability of transition metals to adsorb hydrogen in significant amounts facilitated their practical application. Moreover, this process is reversible, i.e. the decomposition of the formed metal hydrides is accompanied by the release of accumulated hydrogen.

The use of metal hydrides (MH) as reversible hydrogen sorbents opens up prospects for the creation of new multifunctional heat-using devices for energy and technological purposes [1, 2, 3]. Such devices allow performing the operations of receiving hydrogen, its long-term safe storage, purification (including isotope separation), delivery to the consumer with programmable pressure and flow rate, etc.

The processes of storage and purification of hydrogen are based on the phenomenon of sorption. In particular, the process of separation of hydrogen isotopes in the gas - solid system, which occurs when using MH, is based on the phenomenon of adsorption (absorption of a substance from a solution or gas by the surface of a solid). In this case, the formation of the hydride phase of the metal is accompanied by the dissociation of hydrogen molecules on the surface and the incorporation of atoms into the interstices of the crystal lattice.

The study of the equilibria of the phases formed in such systems is not only of theoretical, experimental, but also practical interest in the light of the use of hydrogen. However, such experimental studies are expensive and time-consuming. Therefore, the method of mathematical modeling of phase equilibria in hydrogen - metal hydrides systems has been used recently. This method allows us to restrict experimental studies and it is used in the present work.

Modeling (lattice gas model, dilatation, intermolecular interaction)

Mathematical modeling of the processes occurring during the absorption of hydrogen by metals makes it possible to replace the study of a complex physical process by the study of a similar process on a simplified model. This will allow predicting the data required for the design of metal