Solubility, diffusivity, and permeability of hydrogen at PdCu phases

L.C. Liu, J.W. Wang, Y.H. He, H.R. Gong

www.elsevier.com/locate/memsci

PII: S0376-7388(17)31045-1
DOI: http://dx.doi.org/10.1016/j.memsci.2017.07.057
Reference: MEMSCI15462

To appear in: *Journal of Membrane Science*

Received date: 12 April 2017
Revised date: 24 July 2017
Accepted date: 30 July 2017

Cite this article as: L.C. Liu, J.W. Wang, Y.H. He and H.R. Gong, Solubility, diffusivity, and permeability of hydrogen at PdCu phases, *Journal of Membran Science,* http://dx.doi.org/10.1016/j.memsci.2017.07.057

Solubility, diffusivity, and permeability of hydrogen at PdCu phases

L.C. Liu[a], J.W. Wang[b], Y. H. He[a], H. R. Gong[a*]

[a]*State Key Laboratory of Powder Metallurgy, Central South University, Changsha, Hunan 410083, China*

[b]*College of Physical Science and Technology, Yulin Normal University, Yulin, Guangxi 537000, China*

[*]*Corresponding author. Fax: +86 731 88710855. gonghr@csu.edu.cn*

Abstract

First-principle calculations are used to comparatively investigate solubility, diffusivity, and permeability of hydrogen at body-centered-cubic (BCC) PdCu, face-centered-cubic (FCC) PdCu, and FCC Pd. It is found that solubility of hydrogen at interstitial sites of PdCu and Pd is mainly differentiated by its binding energy and vibration frequency. Moreover, activation energy, instead of jump distance, plays a predominant role in determining hydrogen diffusivity of PdCu and Pd. Calculations also reveal that at a certain temperature, the descending sequence of hydrogen permeability is as follows: FCC Pd→ BCC PdCu→ FCC PdCu, and that the thickness of the membranes fundamentally induces the experimental controversy regarding the relative magnitude of hydrogen permeability of BCC PdCu and FCC Pd. The present results agree well with experimental observations in the literature, and provide a deep understanding to the intrinsic mechanism of hydrogen behaviors in PdCu and Pd.

Keyword: PdCu phases; hydrogen solubility; hydrogen diffusivity; hydrogen permeability; First principles calculation

1. Introduction

The binary PdCu system has been commonly believed as one kind of superior