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Solubility, diffusivity, and permeability of hydrogen at PdCu phasesL.C. Liu^a, J.W. Wang^b, Y. H. He^a, H. R. Gong^{a*}

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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

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