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Texture dependence of hydrogen diffusion in nanocrystalline nickel by atomistic simulations

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ABSTRACT

Atomistic simulations were performed to highlight the importance of the texture on the diffusion of hydrogen atoms in nanocrystalline nickel. Significant anisotropic diffusion is observed in longitudinal and through thickness directions. Our results show that the diffusion coefficient of hydrogen atoms through thickness in [001] textured nickel is larger than those values obtained for [011] and [111]. The diffusivity along longitudinal and transverse directions in [111] textured samples is found to be higher than that along thickness direction. Additionally, it is determined that the presence of hydrogen atoms changes the vacancy formation of the substrate and the vacancy defects are responsible for the anisotropy of hydrogen diffusion. These findings improve our understanding of hydrogen diffusivity at the atomistic level for hydrogen storage in the materials.

Introduction

Hydrogen as a means of energy carrier has been paid considerable attention as an excellent candidate for portable and immobile applications without having negative effect on the environment [1,2]. For examples, fossil fuels can be replaced with hydrogen (carbon-free fuel) in transportation systems [3]. It is expected that hydrogen plays an important role in the evolution of a "clean" source of energy [4]. Hydrogen is a gas at atmospheric conditions, and hydrogen storage as atomic or molecular form is a technological challenge which must be overcome in order to make this source of energy economically [5]. Hydrogen can be stored as (i) liquid at cryogenic temperatures, (ii) gas in pressurized systems, (iii) solid fuel such as metal/complex hydrides (which is physical or chemical combination of hydrogen with materials) [6].

It is possible to store hydrogen in cryogenic or pressurized tanks by modifying the physical state of hydrogen in liquid or gaseous form using the traditional storage methods. On the other hand, due to the low density (0.08988 g/l) and low boiling point (−252.87 °C, at 1 atm) of hydrogen gas, the usual technologies for storage of hydrogen gas are complicated and induced important safety problems for on-board transport applications [1]. As an illustration, to maintain a cryogenic state it is necessary to use a refrigeration unit [7] which raises energy and weight costs and a 40% income loss on the energy content [8]. Also, storage of hydrogen as high pressure gas is restricted due to the weight of the storage container and the possibility for hydrogen leak [1]. Therefore, considerably attempts have been performed on developing of new hydrogen storage systems, such as; carbon nanostructures, chemical hydrides and metal or complex hydrides [9–14]. I. Dincer et al.

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[10] developed new hydrogen production systems from electrolysis to thermo-chemical cycles and from integrated cycles to solar-light based hydrogen production processes. Hydrogen storage by adsorption on carbon materials or absorption as chemical compounds have specific advantages from the viewpoint of safety where, some form of energy input (or transformation) is needed to discharge the hydrogen [9]. Carbon nano-tubes, activated carbons and nano-fibers carbons have been the subject of many researchers due to the high storage capacities in carbon materials [11–13]. S. Z. Mortazavi et al. [14] have studied the effects of different catalysts contacting iron (Fe), molybdenum (Mo), nickel (Ni), cobalt (Co) and their dual compounds with MgO, on hydrogen storage properties of carbon nanostructures containing multi-walled carbon nanotubes and carbon nano-onions. They [14] concluded that various parameters such as vacancy defects, specific surface area and pores (certainly less than 10 nm) of the carbon nanostructures have an influence on the hydrogen uptake and desorption temperature of the stored hydrogen. However, hydrogen storage in carbon nano-materials according to the experimental results scatters over several orders of magnitude [13]. The hydrogen storage capacity of carbon nano-materials is reported between 0.2 and 20 wt % [15]. The experiments to date claiming very high values could not individually be reproduced in various laboratories [1]. Although, carbon nanostructure materials have good reversibility properties, they cannot supply the extent of hydrogen required for automotive applications [15–17].

On the other hand, as the hydrogen atoms can form metal hydrides with some metals or alloys, the solid-state storage of hydrogen can be performed under moderate pressures and temperatures which give them the substantial safety improvement over the conventional storage methods (as liquid and gas). The hydrogen-storage density of metal hydrides are higher (6.5 H atoms/cm^3 for MgH_2) than liquid hydrogen (4.2 H atoms/cm^3) and hydrogen gas (0.99 H atoms/cm^3) [7]. Therefore, the storage of hydrogen as metal hydrides is a free from harm and volume-effective storage method for onboard transportation applications.

Since 1970s various metal-hydrogen alloy systems such as Pd–H have received great attention for developing of clean energy system [18]. As a result, many hydride alloys (metal-hydrogen systems) were studied and developed [19–23]. One of the important studies was the development of rechargeable nickel hydride batteries in 1980s [24]. Nickel hydride batteries have several advantages such as, no environmental pollution problem and memory effect and about twice capacity [24,25].

In currently, hydride composites may be the most effective materials as hydrogen storage alloys for practical utilization in new nickel/metal hydride secondary batteries. S. Pinjari et al. [21] showed that absorption of metallic nickel caused a strong adhesion on MFI structure of ZSM-5 (10%Ni/56.3SiO_2-20.3Al_2O_3) and improvements in textural properties and acid density. Additionally, their results [21] revealed that the addition of nickel on ZSM-5 lead to enhancement in catalyst stability which in turn increase the yields of H_2, carbon nanotubes and conversion to greater values of 3.29%, 4.84% and 90%, respectively.

Storage of hydrogen in metal hydrides depends upon various factors and composed of different mechanism steps. Dissociation of hydrogen by metals depends on their impurity, structure and morphology of surface [26]. Therefore, obtaining better understanding of hydrogen diffusion in metals is a challenge for engineer and scientists in developing of hydrogen economy. The absorption and diffusion of hydrogen in metals depends on the solute atom concentration and the initial microstructure of the substrate (base material) including grain size, grain boundary, interface boundary, misorientation angle, dislocations, triple junctions and texture [27,28]. It is observed that [29] hydrogen diffusion coefficient in nickel decreased from 0.065–0.088 $\times$ 10^{-8} cm^2/s to 0.043–0.048 $\times$ 10^{-8} cm^2/s as the grain size increased from 25 μm to 150 μm. As reported by J. Li et al. [30], the hydrogen diffusion coefficient (D) in nickel single crystals is anisotropy; they obtained values of $D_{\langle 111\rangle} = 15.0 \times 10^{-14}$ m^2/s, $D_{\langle 110\rangle} = 11.0 \times 10^{-14}$ m^2/s and $D_{\langle 100\rangle} = 7.5 \times 10^{-14}$ m^2/s. Cao et al. [31] have measured the hydrogen diffusion in polycrystalline nickel with mean grain size of 3 μm, and obtained $D_{\langle 111\rangle} = 85 \times 10^{-14}$ m^2/s, $D_{\langle 110\rangle} = 65 \times 10^{-14}$ m^2/s and $D_{\langle 100\rangle} = 34 \times 10^{-14}$ m^2/s. Also, P. H. Dederichs et al. [32] have claimed that the anisotropy of the saddle-point structures give rise to an anisotropy in diffusion in cubic crystals. This anisotropy could be an effect of texture or influenced by the nature of grain boundaries. However, the effect of textures on the diffusion of hydrogen atoms in polycrystalline materials with high crystallographic symmetry is less well understood. On the other hand, measure and analyzing of hydrogen distribution in metals and alloys is difficult due to high mobility of hydrogen atoms [33]. The problems of hydrogen detection make it necessary to develop numerical models accounting for physical aspects of hydrogen behavior in metals and alloys [34]. Hydrogen diffusion can be studied theoretically using atomistic simulations, such as first principle calculations [35], molecular dynamics models [36] and so on. Molecular dynamics (MD) simulations give a theoretical approach to study diffusion process. While the accuracy of MD results depends on the inter-atomic potential used in the models, the advantages of MD simulations are that they enable complex atomic structures to be simulated correctly in the computational box, and facilitate the visualization of diffusion mechanisms [37]. While an earlier [31] and recent experimental studies [30] have shown that texture can affect hydrogen permeation in single crystal and microcrystalline nickels, to date there have been few investigations on the effect of initial texture of substrates on hydrogen diffusion through nanocrystalline nickel. For this purpose, in the present paper, the relationship between hydrogen diffusion and textures in nanocrystalline nickel with three different orientations ([001], [110] and [111]) has been studied and different metallurgical parameters which can cause anisotropic diffusivity of hydrogen atoms in nanocrystalline nickel with high crystallographic symmetry crystal lattice (i.e. face centered cubic) have been discussed.

Methodology

Molecular dynamics simulations and inter-atomic potential

Molecular dynamics (MD) simulations were performed using the large-scale atomic/molecular massively parallel simulator

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