Characteristics of New Approach for Aluminum Hydrogen Storage Materials

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***Abstract*—Hydrogen is an effective fuel to overcome the environmental problem. However, hydrogen gas has very small energy per volume and is desired to develop effective way to dense and store hydrogen in a light material. For the purpose of Fuel-Cell Vehicle (FCV), the gravimetric hydrogen content is to be larger than 6 wt%. Aluminum hydride, AlH_3, is hopeful as a hydrogen storage material due to its large gravimetric and volumetric content (10.1 wt% and 148 kg/m^3, respectively). Recently, a new direct-reaction method of synthesizing AlH_3 has been developed under high temperature and pressure [1]. On the other hand, it is a problem that the hydrogenation stops near the interface region between Al and its oxide layers even at high pressure of 10GPa [1]. Our goal is to propose some idea to realize the effective aluminum hydrogen storage material.**

***Index Terms*—hydrogen storage, Aluminum, Fuel cell vehicle,**

I. Introduction

Hydrogen energy research is not only solving environmental issue such as a fossil fuel resources and alternative energy reduction measures, but also tailored for the issues important to the future of the automotive industry are one of the green innovations.

In order to achieve a hydrogen energy systems, and infrastructure development, technology development are important elements relating to the use of hydrogen production, transport and storage [1]-[5].

Because hydrogen is a substance that has the advantage of being compared to the bulk storage of electrical energy.

In order to disseminate the fuel cell vehicles and hydrogen fuel is in fuel cell vehicles, alternative fuel vehicles fuel tank will need a board hydrogen storage system. [6]-[10]

There needs to be improved as a hydrogen refueling infrastructure also temporarily storing hydrogen, the hydrogen with the ability to provide a stable and secure an appropriate speed when the required amount of hydrogen required storage technologies are required.

Therefore, in order to disseminate the energy will be strongly urged to develop hydrogen storage technologies for practical and economical hydrogen. [6]-[16].

II. Experimental Results

A. Fundamental

This research focus on porous alumina AlOx by anodic coating. In Fig. 1, array of nano whole is observed, and it can be controlled by changing the voltage. It should be that the nano whole is used as H-diffusion path. In addition, the presence of thick AlOx layer may change the bonding of H-Al via the image charge of AlOx, and increase H-diffusion. Preliminary experiment results,

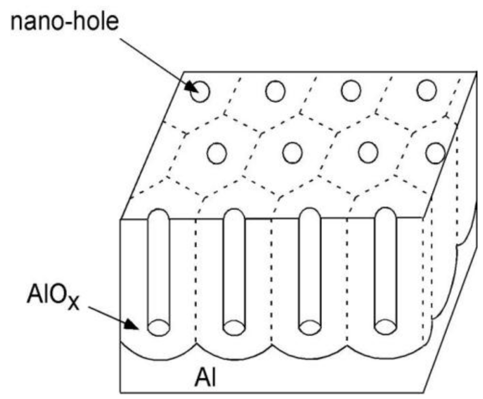

Figure 1. Structure of Porous Alumina/Aluminum by anodic coating [2]

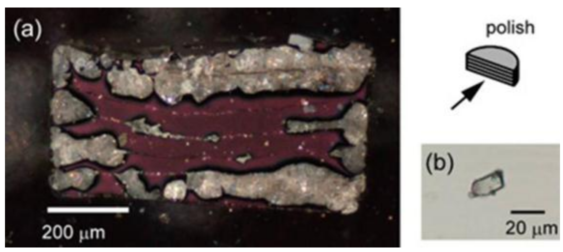

Figure 2. Hydrogenation under high temperature and pressure (Dr. Saito, JAEA) [1]

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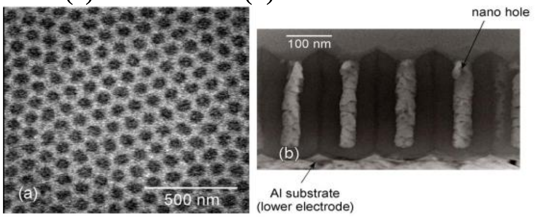
Fig. 2 shows that the thick layer of AlOx facilitates the hydrogenation by SEM, and it takes place more inside of the bulk Al as shown in Fig. 3.

The comparison of experimental results and theory, we tried to understand for the mechanism of slow H-diffusion using ab-initio molecular dynamics (MD). Fig. 4 shows Radial Distribution Function (RDF) for α-AlH_3 crystal at (a) T=100K and (b) T=500K.



(a) SEM Image of Surface (b) TEM Image of Cross Section

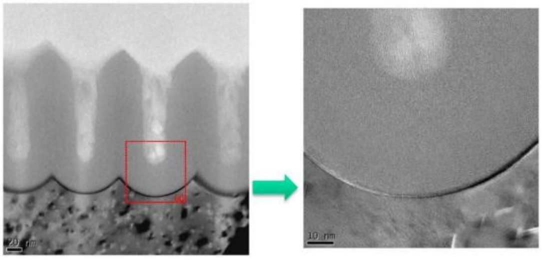
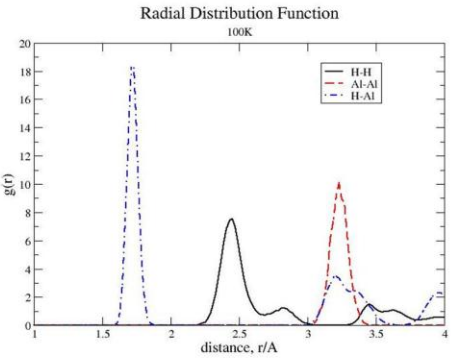
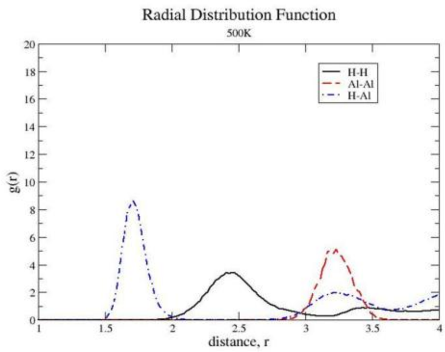


Figure 3. Images of Porous Alumina/Aluminum by anodic coating (Dr. S. Kato, NIMS) [2]



(a) T = 100K



(b) T = 500K

Figure 4. Radial distribution functions of α-AlH3 by ab-initio MD

B. Theory

According to those results, at elevated temperature, H-H and H-Al peaks show broadening. However, H-hoping is not observed. It calculated phonon dispersion and found that the structure is dynamically stable. Hydrogen ordering in Al lattice suppresses H-diffusion and the hydrogenation cannot be developed in whole material. Then, it is important to increase the H-diffusion to utilize whole bulk for effective storage. As increasing temperature, the peak of g(r) increases. However, hydrogen diffusion is not observed. Experimentally, hydrogen does not diffuse after hydrogenation, i.e. AlH3. Then, for the use of whole Al bulk as hydrogen storage, it is important to increase hydrogen diffusion and immerse hydrogen inside the Al bulk before creating AlH_3.

Fig. 5 show the electron density distribution change from atomic states and density of states for Al_2H_3 and Al_2O_3/Al_2H_3. Both peak behaviors shows similar wave. The higher Al_2O_3/Al_2H_3 peak shows around 16 DOS at -7 E/eV however Al_2H_3 shows around 8 DOC at -7 and 0 E/eV.

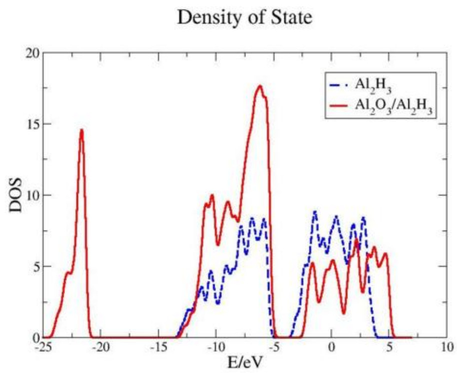
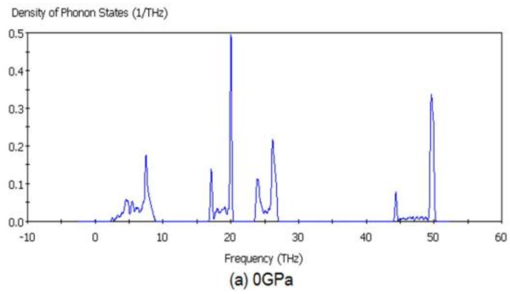


Figure 5. Electron density distribution change from atomic states and density of states for $Al_2O_3/Al_2H_3/Al_2O_3$

Density of ab-initio phonon calculation of α-AlH_3 at (a) 0 GPa and (b) 10Gpa as shown in Fig. 6. According to these results, peak level is almost same except 30THz.



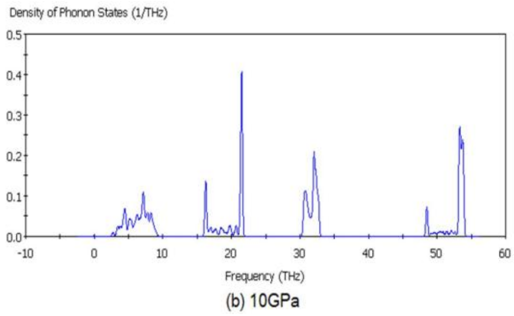
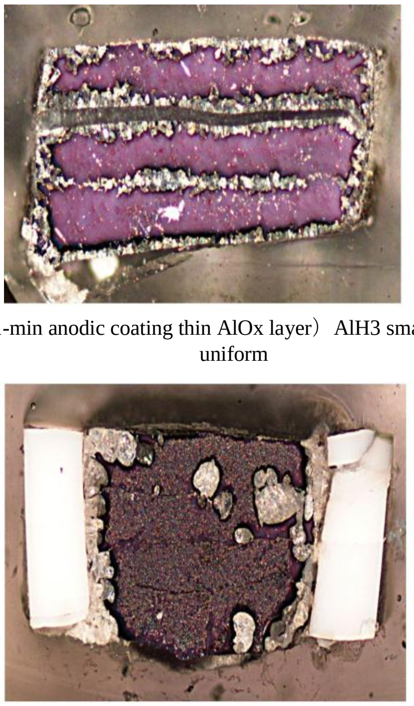


Figure 6. Density of ab-initio phonon calculation of α-AlH_3 at (a) 0 GPa and (b) 10Gpa.

C. *Experiment*

Fig. 7 shows hydrogenated aluminum under high pressure and temperature with alumina layer by SEM image. The 1-min anodic coating thin AlOx layer (a) AlH_3 is small size and uniform, on the other hand, (b) 10-min anodic coating （thick AlOx layer） shows AlH_3 large size and Non-uniform.



(a) 1-min anodic coating thin AlOx layer）AlH3 small size, uniform

(b) 10-min anodic coating （thick AlOx layer）AlH3 large size, Non-uniform

Figure 7. Hydrogenated aluminum under high pressure and temperature with alumina layer by Dr. Saito, JAEA.

Fig. 6 shows that the inside of Al bulk in not hydrogenated under high pressure experiment. This means the Al coated by porous alumina by anodic coating has effect of hydrogen storage more than other materials.

III. CONCLUTION

By alumina layer AlOx, the image charge is induced in Al. Also the Al-H bonding changes from covalent to ionic, and the hydrogen diffusion is increased. It seems nano whole can play as the hydrogen diffusion path. It will be thick AlOx layer to utilize the image charge effect. Therefore it is necessary to do experiment to check the idea continuously.

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