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Mechanical properties of yttrium hydrogen solid solution

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Abstract

The mechanical properties of yttrium hydrogen solid solution (0–0.20 H/Y) were studied to reveal the influence of hydrogen on the characteristics of yttrium. The elastic moduli such as Young's modulus and the shear modulus for yttrium hydrogen solid solution increased with increasing of hydrogen content. The microhardness for the solid solution was also increased with increasing of hydrogen content. The electronic structure of the yttrium hydrogen solid solution was evaluated by a first principle molecular orbital calculation. The mechanical properties of yttrium hydrogen solid solution were discussed in terms of the calculation results.

Keywords: Yttrium hydrogen solid solution; Molecular orbital method; Elastic modulus; Hardness

1. Introduction

Various metal hydrides have attracted much interest as hydrogen storage media. Since the metal hydrides have a high density of hydrogen, some of the metal hydrides are also of interest as the reflectors for fast breeder reactors. In order to apply the metal hydrides as reflectors, properties such as high melting point, low induced activity, small neutron absorption cross-section, low hydrogen desorption pressure, high hydrogen density, phase stability, and cost are desirable. Therefore, it is considered that yttrium hydride is one of the good candidates as reflector. It is known that yttrium absorbs hydrogen up to H/Y = 0.25 and additional hydrogen absorption transforms the yttrium from metal (hcp_A3, α-phase) to hydride (fcc_C1, δ-phase). Although the properties on thin film of yttrium metal or yttrium hydride have been published [1–4], there is inadequate information on yttrium hydrogen solid solution and yttrium hydride for the bulk samples. In the previous works, the authors found that the solute hydrogen deteriorates the mechanical strength of zirconium hydrogen solid solutions [5] and titanium hydrogen solid solutions [6]. However, the effect of solute hydrogen in metals has not been revealed comprehensively. Therefore, it is important to investigate the behaviour of yttrium hydrogen solid solutions. In the present study, bulk yttrium hydrogen solid solutions were fabricated, and the mechanical properties were studied by means of an ultrasonic pulse-echo method and Vickers hardness indentation technique, and the electronic structure was also estimated by a molecular orbital calculation.

2. Experimental procedure

The pure yttrium (99.9%) polycrystalline rectangular column (5 mm × 5 mm × 15 mm) was used as the precursor for fabricating yttrium hydrogen solid solutions in the present study. The hydrogenation of yttrium was executed using a modified Sieverts' UHV apparatus. The details of these conditions were described in our previous paper [7]. The hydrogen content of the specimens was measured by hydrogen analyzer (HORIBA, EMGA-621).

The lattice parameters were obtained on an X-ray diffractometer (RINT-2000/PC, Rigaku Corp.). The ultrasonic pulse-echo measurement gave us the sound velocities and

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elastic moduli (Echometer1062, Nihon Matech Corp.) using the 5.0 MHz ultrasonic waves. The Debye temperatures were estimated from these results. The Vickers hardness was also measured (MHT-1, Matsuzawa Co. Ltd.). The applied load and load time for the indentation were 1.0 kgf and 10 s, respectively.

The electronic structures of the hydrogen solid solutions have been evaluated by a first-principles molecular orbital (MO) calculation. The MO calculations were performed by the DV-Xα cluster method based on the local density function approximation. The DV-Xα method is a non-relativistic first principles method using Slater's Xα potential as the exchange-correlation term. The details of the DV-Xα method have been discussed at length in the literature [8–10].

3. Results and discussion

From the X-ray diffraction patterns it was found that all of the samples prepared in the present study showed an hcp_A3 (α) single phase. The lattice parameters a, c at room temperature are plotted as a function of the hydrogen content C_H in Fig. 1. It is found from this figure that the lattice parameter slightly increases with increasing hydrogen content, according to the following relationship:

$$a\,(\mathrm{nm}) = 0.3646 + 1.029 \times 10^{-2} \times C_H(\mathrm{H/Y}) \quad (1)$$

$$c\,(\mathrm{nm}) = 0.5722 + 3.363 \times 10^{-2} \times C_H(\mathrm{H/Y}) \quad (2)$$

The present results were almost as same as the results in other reports [11–13]. The linear expansion coefficient of the c-axis on the hydrogen content, $\lambda_c = (1/c)(\partial c/\partial C_H)$ is 3.36×10^{-2}, which is larger than the coefficient of the a-axis, $\lambda_a = (1/a)(\partial a/\partial C_H)$ is 1.03×10^{-2}. It is considered that this difference is due to the fact that the actual c/a ratio for yttrium (1.57) is smaller than the ideal ratio for an hcp structure ($\sqrt{8/3}$). It was also found that the real densities of the samples were approximately equal to the theoretical density calculated from the lattice parameter.

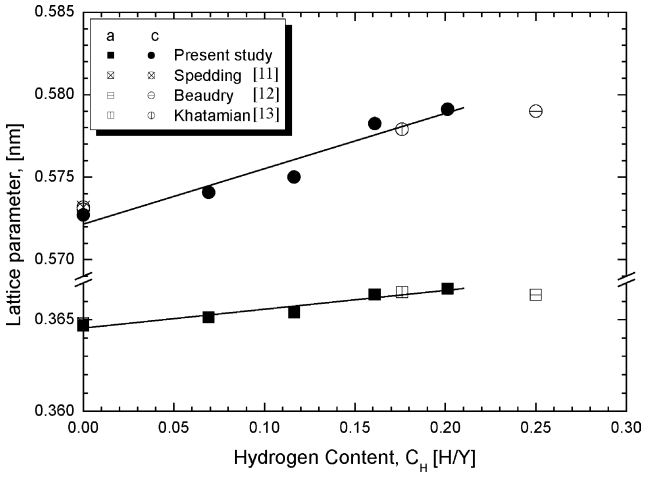

Fig. 1. Change in the lattice parameters a and c for yttrium hydrogen solid solution with hydrogen content C_H, together with the lines calculated from Eqs. (1) and (2).

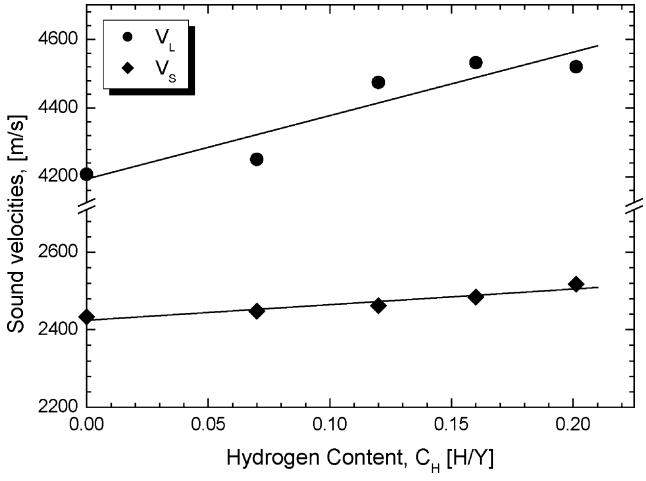

Fig. 2. Change in the sound velocities V_L and V_S for yttrium hydrogen solid solution with hydrogen content C_H, together with the lines calculated from Eqs. (3) and (4).

Fig. 2 shows the change in the ultrasonic sound velocities for yttrium hydrogen solid solutions with hydrogen content. Both the longitudinal and the shear sound velocities increased with hydrogen addition and can be expressed as follows:

$$V_L\,(\mathrm{m/s}) = 4193.3 + 1847.8 \times C_H(\mathrm{H/Y}) \quad (3)$$

$$V_S\,(\mathrm{m/s}) = 2424.5 + 404.2 \times C_H(\mathrm{H/Y}) \quad (4)$$

Young's modulus E, the shear modulus G, the bulk modulus B, Poisson's ratio ν and the Debye temperature θ_D are calculated from the longitudinal velocity V_L and the shear velocity V_S as follows:

$$E = \rho V_S^2 \left\{ \frac{3V_L^2 - 4V_S^2}{V_L^2 - 4V_S^2} \right\} \quad (5)$$

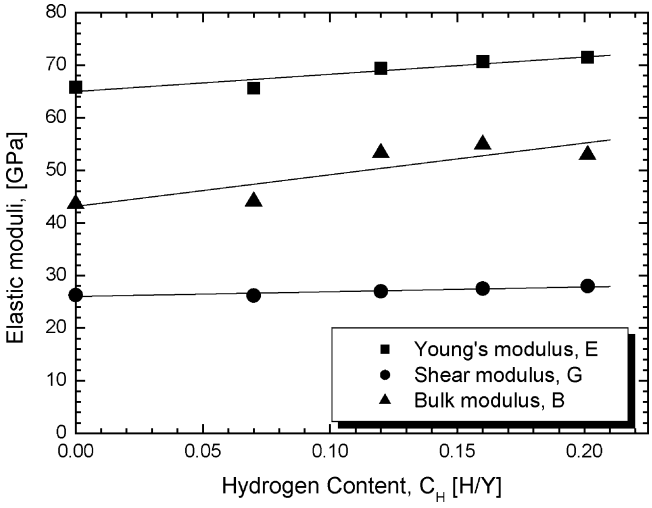

Fig. 3. Change in the elastic moduli for yttrium hydrogen solid solution with hydrogen content C_H, together with the lines calculated from Eqs. (9)–(11).