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Thermal properties of yttrium hydride

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Abstract

The thermal properties of δ-phase yttrium hydrides (YH_x: $x = 1.72$–2.00) were studied in the temperature range from 300 to 773 K. The heat capacities of yttrium hydrides are larger than that of yttrium metal because of hydrogen optical vibration. The thermal conductivities of the yttrium hydrides are larger than that of metal and have strong dependence on temperature. They are not markedly influenced by the hydrogen content.

1. Introduction

Metal hydrides are very attractive and important materials in the nuclear energy field. In particular the yttrium hydride is significantly stable at high temperature, therefore it is expected to be used as material for weakening neutron energy spectrum of the fast reactor. However, various properties of yttrium hydride are hardly known and there are very few reports about them. This is attributed to the fact that metal hydrides are cracked or pulverized in a usual fabrication process. In our previous study, the zirconium and titanium hydrides were fabricated without flaw, and then the various properties of them were measured [1,2]. From this knowledge, we can find the way to fabricate flaw-free yttrium hydride. In this paper, the thermal properties of the yttrium hydrides were studied.

2. Experimental procedure

δ-Phase yttrium hydride samples were prepared in a modified Sieverts' apparatus. We have succeeded in fabricating flaw-free bulk samples of yttrium hydrides. The preparation process was reported in our previous paper [3]. The heat capacity was measured in the temperature range from 323 to 773 K by a differential scanning calorimeter (Triple-cell DSC, ULVAC-RIKO Inc.). The thermal diffusivity was measured using a laser flash apparatus (TC-7000, ULVAC) from 300 to 773 K in vacuum. The thermal conductivity was calculated from the thermal diffusivity, the heat capacity and the density.

3. Results and discussion

Fig. 1 shows the heat capacities C_p of pure yttrium and δ-phase yttrium hydrides as a function of temperature T. In this study, the dependence on hydrogen content was not observed. The heat capacity of YH_x is expressed as follows:

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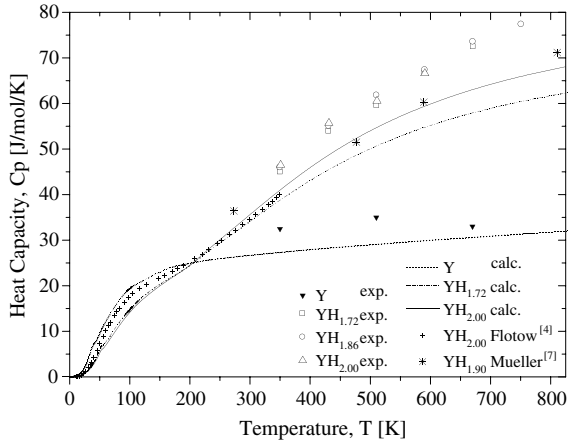

Fig. 1. The heat capacities C_p of the yttrium and the yttrium hydrides.

$$C_p = 37.28 + 5.707 \times 10^{-2} \times T + 1.391 \times 10^{6} \times T^{-2}. \quad (1)$$

From the experimental and literature [3–5] data, we can estimate various contributions to the heat capacity of yttrium hydride: the contributions are the metal vibrational term for the acoustic mode, the dilatational term, the electronic term and the hydrogen vibrational term for the optical mode. The details of the calculation were described in our previous paper [6]. The total values were also drawn as curves in Fig. 1. These calculated heat capacities were slightly smaller than the experimental results obtained in the present study. Above room temperature, the heat capacities of yttrium hydrides were much larger than that of the yttrium metal. The calculation indicated that they are attributable to the optical phonon due to hydrogen vibration.

Fig. 2 shows the thermal diffusivities α of the yttrium hydride (YH_x: x = 1.72, 1.86, 1.90) as a function of temperature. The thermal diffusivities of the hydrides are larger than that of the metal in the temperature range from room temperature to 700 K. This characteristic becomes much more pronounced as temperature decreases.

The thermal conductivity κ is derived from the thermal diffusivity α, the heat capacity C_p, and the density ρ:

$$\kappa = \alpha C_p \rho. \quad (2)$$

The densities ρ of $YH_{1.72}$ and $YH_{1.86}$ and $YH_{1.90}$ were 4.24, 4.26 and 4.27 g/cm^3 respectively which were determined from weight and dimensional measurements. Fig. 3 shows the estimated thermal conductivities of the yttrium hydrides, which are larger than that of metal. There is significantly difference between the present study and literature [7]. However we do not have enough details for the measurements of [7] to assess the origin of the difference. As with the diffusivities, the thermal conductivities of the hydrides decrease with temperature increase, whereas that of metal remains almost constant with a slight dependence on the hydrogen content being observed.

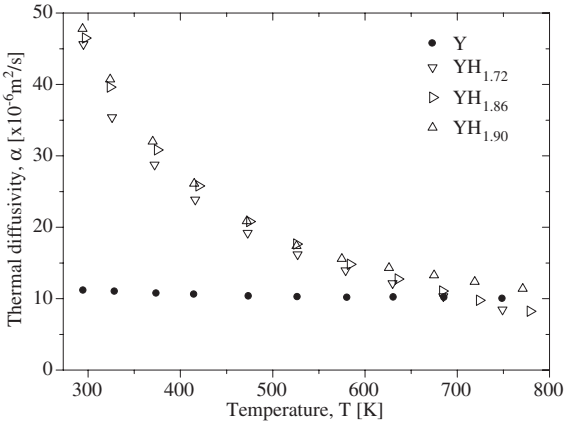

Fig. 2. The thermal diffusivities α of the yttrium and the yttrium hydrides.

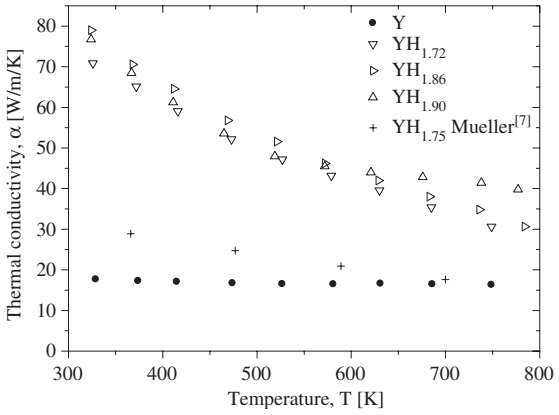

Fig. 3. The thermal conductivities κ of the yttrium and the yttrium hydrides.

The total thermal conductivity can be represented as the sum of the electron (κ_{el}) and phonon (κ_{ph}) components: $\kappa_{total} = \kappa_{el} + \kappa_{ph}$. The electron contribution was estimated with the use of the Wiedemann–Franz relationship $\kappa_{el} = \sigma LT$: L and σ are the Lorentz number and the electrical conductivity, respectively. The electrical conductivities of the yttrium hydrides were also measured and the results will be reported in the future [8]. The phonon contribution κ_{ph} was estimated by subtracting κ_{el} from κ_{total}. As shown in Fig. 4, both κ_{el} and κ_{ph} of hydride are larger than those of metal, respectively. The increase of κ_{el} for hydride against metal is attributed to the increase of electrical conductivity. It is considered that the difference of κ_{ph} between the hydride and metal is caused by the difference of the Debye temperature [3].

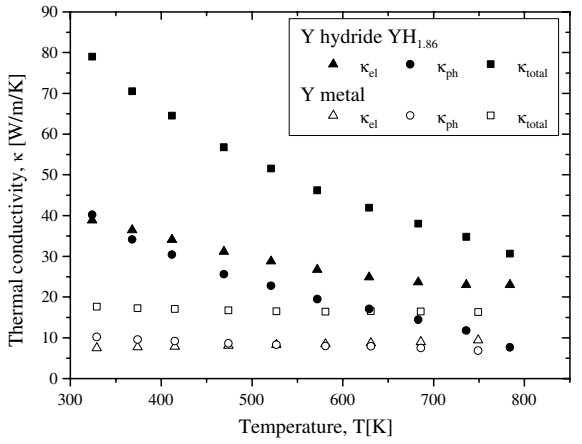

Fig. 4. The contributions of the electrons and phonons for the thermal conductivities.

The thermal conductivities of zirconium hydride and titanium hydride [1,9] show a nearly constant value of 20 W/m/K against T. Therefore yttrium hydride is superior to zirconium hydride and titanium hydride in regard of heat removal.

4. Conclusions

The single δ phase yttrium hydride (YH_x: $x = 1.72$–2.00) specimens were fabricated directly from bulk yttrium metal without cracks. Thermal properties of the yttrium hydrides were studied. The heat capacities of the hydrides were larger than that of metal. These results are qualitatively understood as the effect of optical mode by the hydrogen vibration. The thermal conductivities of the hydrides were strongly dependent on temperature but slightly dependent on the hydrogen content.

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