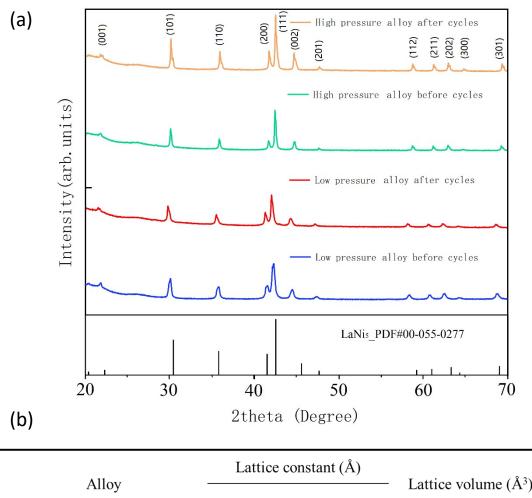
Electronic supplementary information (ESI)

## Temperature rise of LaNi<sub>5</sub>-based alloys by hydrogen absorption

Nanxu Zhou<sup>a</sup>, Masakuni Yamaguchi<sup>b</sup>, Hiroki Miyaoka<sup>b</sup> and Yoshitsugu Kojima\*<sup>b</sup>

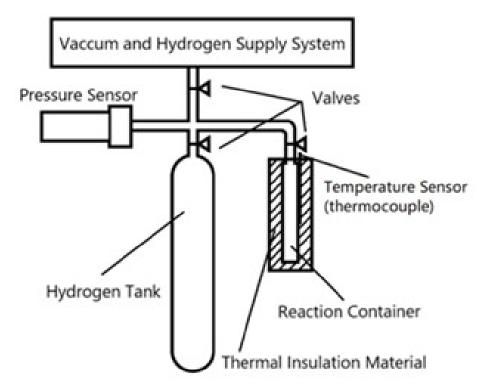
 <sup>a</sup> Graduate School of Advanced Sciences of Matter, Hiroshima University, 1-3-1, Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8530, Japan
<sup>b</sup> Natural Science Center for Basic Research and Development, Hiroshima University, 1-3-1, Kagamiyama, Higashi-Hiroshima, Hiroshima 739-8530, Japan

\* Corresponding author. Tel.: +81 82 424 3904; fax: +81 82 424 5744. *E-mail address:* kojimay@hiroshima-u.ac.jp (Y. Kojima).



Alloy			Lattice volume ( $A^3$ )
	$a_0$	$c_0$	
High pressure alloy-before	5.01	3.99	86.53
High pressure alloy-after	4.99	4.03	86.92
Low pressure alloy-before	5.02	4.07	89.03
Low pressure alloy-after	5.02	4.08	89.17

Fig. S1 (a) XRD patterns before and after hydrogen storage cycles of the AB<sub>5</sub>-type alloys as purchased, which is  $La_{0.803}Ce_{0.140}Pr_{0.0148}Nd_{0.0427}Ni_{3.99}Co_{0.61}Mn_{0.30}Al_{0.27}$  (referred as low-pressure AB<sub>5</sub> alloy ),  $La_{0.241}Ce_{0.543}Pr_{0.0538}Nd_{0.163}Ni_{3.986}Co_{0.601}Mn_{0.360}Al_{0.053}$  (referred as high-pressure AB<sub>5</sub> alloy ) together with the data of  $LaNi_5$  (JCPDS file No. 00-055-0277). XRD indicates that low-pressure AB<sub>5</sub> alloy and high-pressure AB<sub>5</sub> alloy have hexagonal CaCu5-type crystal structure, and the crystal structures will not change due to hydrogen storage. (b) The lattice constants and cell volume of the presented alloys, the lattice experienced an expansion after cycles



**Fig. S2** Conceptive picture of specially designed heat generation rate measurement apparatus. A thermocouple was attached on the surface of the vessel to record the surface temperature. A big hydrogen tank was used to maintain sufficient operating pressure.

Materials	Data source	
$H_2, CH_4, NH_3, water, C_4 OH,$ Methylcyclohexane, Toluene, CCl <sub>4</sub>	NIST chemistry webbook <sup>1</sup>	
N-Octane, Benzene	Literature <sup>2</sup>	
NbH <sub>2</sub> , PdH <sub>0.7</sub> , LaNi <sub>5</sub>	Literature <sup>3</sup>	
MgH <sub>2</sub>	Literature <sup>4</sup>	
LiH	Literature <sup>5</sup>	
Low-pressure $AB_5$ alloy, high-pressure $AB_5$ alloy	By authors	
LaNi Sn 4.8 0.2	Literature <sup>6</sup>	

Fig. S3 Table of the data source in Fig.5 and Fig.6

## References

- J. S. C. William E. Acree, Jr., in NIST Chemistry WebBook, NIST Standard Reference Database Number 69, Eds. P.J. Linstrom and W.G. Mallard, National Institute of Standards and Technology, Gaithersburg MD, 20899, 2021.
- 2 S. T. BOWDEN, *Nature*, 1954, **174**, 613–614.
- 3 T. Schober and H. Wenzl, *Hydrogen in metals II*, 1978.
- 4 A. San-Martin and F. D. Manchester, J. Phase Equilibria, 1987, 8, 431–437.
- 5 E. Veleckis, E. H. Van Deventer and M. Blander, 1974, **78**, 1933–1940.
- 6 S. Luo, W. Luo, J. D. Clewley, T. B. Flanagan and R. C. Bowman, *J. Alloys Compd.*, 1995, **231**, 473–478.