Effect of hydrogenation on the local structures around Ni and La in LaNi₅

Makoto MATSUURA¹*, Kazuya KONNO ¹, Kaku ASADA¹ and Masaki SAKURAI²
¹Miyagi National College of Technology, Nodayama Natori, Miyagi 981-1239, Japan
²Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Introduction
The combination of the easy-hydride-forming element of La and the hard-hydride-forming element of Ni in LaNi₅ lowers the formation energy of hydride. Theoretical calculation using DV-Xα suggests that protium in LaNi₅ preferentially interacts with Ni rather than La[1]. Therefore, XAFS spectrum is expected to show that the Debye temperature of Ni will be strongly affected by hydrogenation. In the present work we measured XAFS of the La L-edge and Ni K-edge for LaNi₅ and LaNi₅H₆ at various temperatures from 20 to 300K. In this report the temperature dependences of χ(k) of the L₃ edge of La and K-edge of Ni only for LaNi₅ are reported.

Experiments
The Sample of LaNi₅ is prepared by arc melting. The sample of LaNi₅H₆ is prepared by hydriding LaNi₅ at 353K under 4.3 MPa H₂ gas. The structures of LaNi₅ and LaNi₅H₆ are confirmed by X-ray diffraction. Special attentions to the sample holder are paid to prevent desorption of hydrogen from LaNi₅H₆ sample during evacuation in the cooling process.

XAFS measurements of the La L₃ edge and Ni K-edge are done at temperatures of 20K, 100K, 200K and 300K using Si(111) monochromator. UWXAFS program is used for data analyses (AUTOBK) and XAFS calculation (FEFF).

Results and Discussion
χ(k) curves and their Fourier transforms of the La L₃ edge and Ni K-edge for LaNi₅ at various temperatures are shown in Figs. 1-4 together with the calculated one using FEFF. Though quantitative analysis is not accomplished yet, temperature dependence of radial structure function F(r) is more pronounced for La than Ni.

The agreement with calculated results is fairly good except beyond 0.6nm. More precise analysis and the results for LaNi₅H₆ will be reported soon.

References
*matsuura@miyagi-ct.ac.jp