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Effect of hydrogenation on the local structures around Ni and La in $LaNi_5$

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Introduction

The combination of the easy-hydride-forming element of La and the hard-hydride-forming element of Ni in $LaNi_5$ lowers the formation energy of hydride. Theoretical calculation using DV-X_α suggests that protium in $LaNi_5$ 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 $LaNi_5$ and $LaNi_5H_6$ at various temperatures from 20 to 300K. In this report the temperature dependences of χ(k) of the L_3 edge of La and K-edge of Ni only for $LaNi_5$ are reported.

Experiments

The Sample of $LaNi_5$ is prepared by arc melting. The sample of $LaNi_5H_6$ is prepared by hydriding $LaNi_5$ at 353K under 4.3 MPa H_2 gas. The structures of $LaNi_5$ and $LaNi_5H_6$ are confirmed by X-ray diffraction. Special attentions to the sample holder are paid to prevent desorption of hydrogen from $LaNi_5H_6$ sample during evacuation in the cooling process.

XAFS measurements of the La L_3 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 L_3 edge and Ni K-edge for $LaNi_5$ 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.

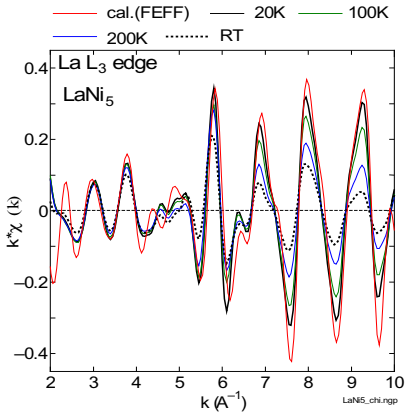

Fig. 1 χ(k)*k vs k curves of the La L_3 edge for $LaNi_5$ at various temperatures together with the calculated using FEFF

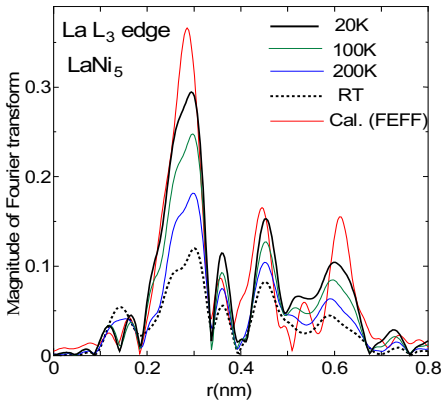

Fig.2 Fourier transforms of the χ(k)*k for $LaNi_5$ at various temperatures together with the caluculated using FEFF

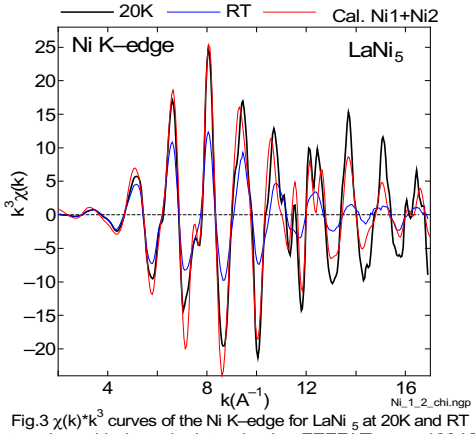

Fig.3 χ(k)*k^3 curves of the Ni K–edge for $LaNi_5$ at 20K and RT together with the calculatged using FEFF(T_{Debye} =180 K)

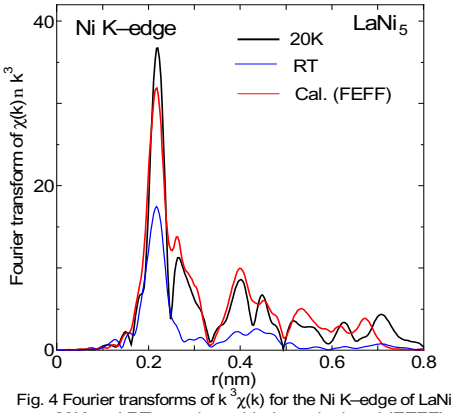

Fig. 4 Fourier transforms of $k^3\chi$(k) for the Ni K–edge of $LaNi_5$ at 20K and RT together with the calculated (FEFF)

The agreement with calculated results is fairly good except beyond 0.6nm. More precise analysis and the results for $LaNi_5H_6$ will be reported soon.

References

[1] H. Yukawa et al., Intermetallics 4, S215 (1996).

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