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MAGNETIC AND CRYSTALLOGRAPHIC PROPERTIES OF $LaNi_{(5-x)}Fe_x$

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Rare earth-iron intermetallics are still the best candidates for the next generation of economically feasible high performance permanent magnetic materials. In spite of several decades of research dedicated to understanding the magnetic interactions in these materials, several aspects remain poorly understood. Recent developments[1] in spin resolved photoemission spectroscopy provide an opportunity to investigate, in unprecedented detail, a poorly understood aspect, the relationship between the electronic band structure and the bulk and microscopic magnetic properties. However, interpretation of spin-resolved photoemission spectra of complex intermetallics is very difficult. Consequently, it is prudent to first study a relatively simple system such as RM_5 (*R*-rear earth, M-transition metal), which is the building block of more complex intermetallics such as RM_{12} and R_2M_{17}. Because RFe_5 intermetallics do not exist, one must study an iron doped RM_5 system such as $LaNi_{(5-x)}Fe_x$ in order to obtain information about the contribution from the iron sub-lattice to the band structure.

For best results, it is desirable to study samples with large amounts of iron. Iron concentrations of samples used in early studies[2] of $LaNi_{(5-x)}Fe_x$ were limited to about x=1.2 but concentrations as high as x=1.5 have been recently achieved[3] using somewhat tedious processing techniques. Herein, we report the crystallographic and magnetic properties of a series of induction melted $LaNi_{(5-x)}Fe_x$ ($0 \le x \le 1.4$) samples intended for spin-resolved photoemission analysis. The information presented in this paper will be crucial to the success of the planned spin-resolved photoemission studies.

$LaNi_{(1-x)}Fe_x$ samples were prepared from 99.99 percent pure elements by induction melting in a cold copper crucible followed by annealing at 950°C for 120 hours. The phase purity of the samples was checked by x-ray diffraction with Cu K_α radiation on a Scintag XDS 2000 x-ray diffractometer equipped with a single crystal graphite monochromator. The bulk magnetic properties of the samples were measured at the Southern Illinois University-Carbondale on a Quantum Design SQUID magnetometer. The powder neutron diffraction data were obtained at the University of Missouri Research Reactor for samples placed in thin-walled vanadium containers and exposed to 1.4875 Å neutrons for 4-6 hours each at 30 and 295 K. The spectra were refined by the Rietveld technique.

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Figure 1 shows thermo-magnetic data for three of the samples. The data for x=1 and for x=1.2 sample are in good agreement with prior work.[2] Increasing the iron content from x=1.2 to x=1.35 increases the Curie temperature by another 25 degrees. However, saturation magnetization is affected only marginally by the same change in the iron concentration.

Neutron diffraction patterns for all of the samples could be fit based on the $CaCu_5$ type structure (space group P 6/mmm). Figure 2 shows the neutron diffraction pattern measured at 30 K for $LaNi_{3.65}Fe_{1.35}$ along with a fit based on the $CaCu_5$ type structure. The unit cell expands isotropically with increasing iron content such that the cell volume of $LaNi_{3.65}Fe_{1.35}$ is 3.4% larger than that of $LaNi_5$. Refined occupancy factors indicate that approximately 90% of the iron atoms occupy the 3g transition metal site.

Analysis of bulk magnetization data and magnetic moments obtained from neutron diffraction data reveals that Ni atoms posses a induced magnetic moment.

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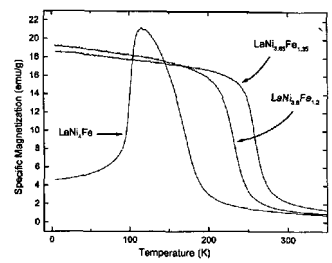

Fig. 1. Thermo-magnetic data for selected $LaNi_{(5-x)}Fe_x$ samples.

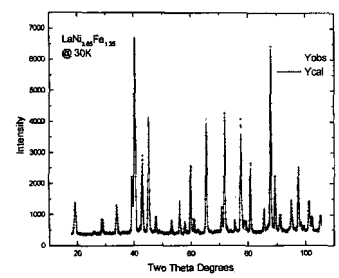

Fig. 2. Neutron diffraction pattern measured at 30 K for $LaNi_{3.65}Fe_{1.35}$ and a fit based on the $CaCu_5$ structure.

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