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PROGRESS REPORT

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FUNDAMENTAL STUDIES OF NEW HIGH-ENERGY PERMANENT MAGNET MATERIALS

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Rare-earth transition metal nitrides and carbides have been prepared by gas-solid reaction with nitrogen and hydrocarbon gases. Crystal structure studies indicate that the original structures are retained with carbon uptake, while the lattice is expanded by the interstitial carbon atoms. The average expansions of the unit cell volume are 7.5% for R_2Fe_{17} and about 1.5 - 3.0% for $R(Fe,M)_{12}$ compounds, resulting in a drastic increase of Curie temperature. In R_2Fe_{17}, T_c increases by about 284 to 400 K through the ethane treatment. The Curie temperature of the $R(Fe,M)_{12}$ alloys, however, typically increases by 150 to 200 K. Spontaneous magnetization was also raised by the carbon uptake. This increase is rather large at room temperature because of the low Curie temperature of the parent alloys.

Neutron diffraction has been used to study the changes in structure which accompany the nitrogenation. While some of these, like the change in lattice constants and cell volume can also be determined by x-ray diffraction, the other changes, including nitrogen location and occupation, and interatomic bond lengths can only be determined by Rietveld analysis of neutron data. It has been found that in $NdFe_{10}Mo_2N_x$ nitrogen occupies the base center site (½, ½, 0) of the tetragonal unit cell with 84% occupancy. Mo atoms are found to populate the Fe site at 0.3607, 0, 0 which is quite different from the V compounds (x, ½, 0).

Two types of crystal structure have been found in $LaFe_{13-x}Si_x$ compounds; the face-centered cubic $NaZn_{13}$-type phase which occurs for $x \leq 2.4$ and the body-centered tetragonal $Ce_2Ni_{17}Si_9$-type structure for $3.5 \leq x \leq 5.0$. Nitrogenation of samples with the cubic phase expanded the unit cell by 6.2 to 10.8%. The lattice expansion led to increases in Curie temperature (52 to 80K) and spontaneous magnetization (around 10%). Unlike the cubic phase,

however, the tetragonal phase was not significantly affected by the nitrogenation.

The interstitial nitrogen atom introduced by nitrogenation in a nitrogen gas atmosphere expanded the unit cell volume of $NdFe_{10}Mo_2$ compound by about 3%. The Curie temperature of the nitride reached 563 K. The magnetic anisotropy field was increased to 20 and 8.6 T at 10 and 300 K, respectively, and this makes this compound a prospective permanent magnet. Magnetically hard $NdFe_{10}Mo_2N_x$ with coercivity of 8.8 kOe at room temperature and 33.7 kOe at 10 K were obtained by nitrogenating the melt-spun $NdFe_{10}Mo_2$ ribbons. It was found that the coercivity depends strongly on the nitrogenation temperature and time with a maximum at 570 °C for 4 hours. The high coercivity is related to the purity of the $ThMn_{12}$ phase and the uniformity of nitrogenation. The $ThMn_{12}$ structure was retained after nitrogenation with only 5% of free iron as the impurity. The nitrogen content was very close to the saturation value, indicating a fairly uniform nitrogenation throughout the particles.

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