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STRUCTURAL STUDIES OF RARE EARTH-IRON NITRIDES BY NEUTRON POWDER DIFFRACTION

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New high performance permanent magnets have been found as the result of nitrogenation of rare-earth-iron-based phases, including RE_2Fe_{17} and $REFe_{12-x}TM_x$ where TM is a transition-metal such as Mo, V, Al, Ti. We have used neutron diffraction to study the changes which accompany the nitrogenation in a number of these compounds, including Y_2Fe_{17}, Nd_2Fe_{17}, $NdFe_{10}Mo_2$ and $NdFe_{10}V_2$.

In the RE_2Fe_{17} systems, the nitrogen atoms are found to occupy the largest interstitial site, the h site in Y_2Fe_{17} and the equivalent e site in Nd_2Fe_{17}. There are indications of a second interstitial site with a low nitrogen occupancy. The primary sites are found to be less than fully populated, perhaps due to steric constraints, since the Fe-N bonds are relatively short. In $Nd_2Fe_{17}N_x$, there are clear indications of variable nitrogen filling.

In the $RETM_{12}$ systems, the nitrogen is found only in the large interstitial site at $0\,0\,\frac{1}{2}$, and depending on preparation, this site may approach full occupancy. The cell volume is found to vary with the nitrogen filling, and intermediate nitrogen occupancies are observed.

The change in interatomic distances has been examined across these compounds. We find that the Curie point follows a nearly linear relationship with the average Fe-Fe bond length for the Nd_xFe_y compounds investigated including $Nd_2Fe_{14}B$. A relationship between anisotropy direction and average Nd-Fe bond length is also noted.

The data also emphasize the difficulty of producing high quality samples with uniform composition, low strain and reasonable particle size. The samples which meet these criteria are those which give the best refinement results and which can provide definitive answers to the basic properties of these exciting new materials.

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