Origin of Fe substitutions in $Nd_2Fe_{17-\delta}X_\delta$

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In $Nd_2Fe_{17-\delta}X_\delta$ ($X=$ Al, Si, Ti, V, Cr, Mn, Co, Ga, Nb, Mo, W, and $\delta=0,\ 0.5$) the X atoms substitute for Fe without changing the crystal structure. Neutron-diffraction measurements show that Al, Si, Co, and Ga tend to substitute for Fe with a strong preference for the $18h$ sites while Ti, V, Cr, Mn, Nb, Mo, and W tend to substitute for Fe with a strong preference for the $6c$ sites. This substitution can be understood by considering a model which includes contributions from the enthalpy of solution of the X atom at each Fe site, the elastic energy due to the differences in the volume of the site and the volume of the X atom, and a structural-dependent contribution reflecting the difference in the average number of valence electrons at each Fe site. [S0163-1829(98)09809-9]

The R_2Fe_{17} ($R=$ rare earth) compounds have the highest magnetization among all R-Fe binary compounds. The light rare earths (Ce to Tb) form the rhombohedral Th_2Zr_{17} structure, and the heavy rare earths (Dy to Lu) and Y form the hexagonal Th_2Ni_{17} structure. However, they are not suitable as permanent magnet materials because of their low Curie temperatures T_C and basal-plane anisotropy at room temperature. In order to improve the magnetic properties of R_2Fe_{17}, Fe was substituted by various metallic elements. The results[1,2] showed that both higher T_C and uniaxial anisotropy can be obtained by substituting some of these elements for Fe in Sm_2Fe_{17}. In Nd_2Fe_{17}, isostructural with Sm_2Fe_{17}, Nd occupies one crystallographic site $6c$, while Fe occupies four different crystallographic sites, $x=6c$, $9d$, $18f$, and $18h$. The observed changes in the magnetic properties are closely related to nonrandom substitution in the Fe sites. Therefore, for modeling the magnetic properties of R_2Fe_{17} it is essential to understand the *driving force* behind the Fe substitution in order to predict the site position of the Fe-substituting element. This could be of great interest in improving the magnetic properties in R-Fe compounds as well as in ternary R-Fe-B compounds where nonrandom Fe substitution has already proven to be necessary for obtaining optimal magnetic properties in these materials.

Neutron-diffraction techniques[3–8] have been used in order to determine the position of the X atoms in $Nd_2Fe_{17-\delta}X_\delta$. The results show that the X atoms preferentially substitute for Fe in the $6c$ or $18h$ sites in Nd_2Fe_{17}.[3–8] Co and Nb are also found to substitute for Fe in the $9d$ and $18f$ sites in Nd_2Fe_{17}, respectively.[3,5] There is no unique explanation for the observed substitutions. Both the chemical affinity and the size effect were suggested to play a role in the Fe substitution. Moreover, to date, no *quantitative* explanations are available to interpret all the results. In this paper we present a model for calculating the occupation probabilities for each Fe site for all substituent atoms and compare them with experimental results.

The details of sample preparation and neutron-diffraction measurements and analyses were presented previously.[6,7] All measurements were done at 380 K (420 K for Co), above T_C, to avoid the contribution from magnetic scattering and allow us to fit only the structural parameters. In Refs. 6–8 we have assumed isotropic thermal vibration factors U_{iso} and constrained all Fe atoms, irrespective of site, to have the same value of U_{iso}. However, the quality of the fits was noticeably improved by considering different U_{iso} for each Fe site. The ratios of U_{iso}, however, for different sites in $Nd_2Fe_{17-\delta}X_\delta$ were kept identical to those corresponding to the unconstrained factors in Nd_2Fe_{17} at the same temperature. At 380 and 420 K the ratio of U_{iso} of Fe sites in Nd_2Fe_{17} is $U_{iso}(6c):U_{iso}(9d):U_{iso}(18f):U_{iso}(18h) = 1.29:1:1.30:1.15$. The resulting occupations do not vary significantly from those published previously,[6–8] and are given in Table I. The neutron-diffraction measurements show that all the samples, except for $X=$ Nb, were of single 2-17 phase with about 1% of α-Fe. For $X=$ Nb, in addition to the 2-17 phase a few percent of the $NbFe_2$ phase was also present. For comparison purposes, all the fitting results in Table I were normalized to $\delta=0.5$. Our results are in good agreement with those of Refs. 3, 4, and 5. We did not, however, observe the preferential occupation of Co and Nb in the $9d$ and $18f$ sites, respectively.

All substituted atoms except Co have larger metallic radii than Fe, 1.26 Å. Table I shows that only for the $9d$ site does the occupation of the X atoms depend on the atomic size; X atoms larger than Mn (i.e., ≥ 1.32 Å), do not occupy the $9d$ site. A small percentage of the X atoms are found in the $18f$ site. The $6c$ and $18h$ sites are the only sites that have *preferential* occupancies, i.e., occupancies higher than that expected from a random distribution of the X atoms over all Fe sites, $\delta/17$ or 2.94%. These two sites have significantly different environments than the other two sites. The $6c$ site has the smallest number of Nd and the largest number of Fe nearest neighbors while the $18h$ site has the largest number of Nd and the smallest number of Fe nearest neighbors. Also, the $6c$ site and $18h$ site have larger Wigner-Seitz volumes than the $18f$ and $9d$ sites. It is clear that the volume and the environment of the Fe sites must be considered in any model that provides quantitative results for the occupancies of the X atoms in Nd_2Fe_{17}. The Wigner-Seitz volume of the Fe sites increases proportionally with temperature,[6] hence, we can assume that in the temperature range where the

TABLE I. Experimental and calculated values of fractional site occupations of the X atoms in each x site in $Nd_2Fe_{16.5}X_{0.5}$.

| X_δ | $Al_{0.5}$ | | $Si_{0.5}$ | | $Ti_{0.5}$ | | $V_{0.5}$ | | $Cr_{0.5}$ | | $Mn_{0.5}$ | |
Fe sites	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.
$\%X,6c$	0.5(8)	3.1	0	2.2	21.4(4)	23.8	19.6(5)	20.4	11.8(8)	13.5	6.9(3)	6.7
$\%X,9d$	0	1.2	2.2(8)	1.3	0	0.3	0	1.1	0	2.3	0.8(3)	2.2
$\%X,18f$	1.7(4)	2.7	1.1(5)	2.8	0.7(2)	0.2	1.2(3)	0.8	2.6(4)	1.9	2.4(2)	2.7
$\%X,18h$	6.5(4)	4.0	6.2(5)	4.1	0.5(2)	0	0.6(3)	0.2	1.8(4)	0.7	3.1(2)	2.3

| X_δ | $Co_{0.5}$ | | $Ga_{0.5}$ | | $Nb_{0.5}$ | | $Mo_{0.5}$ | | $W_{0.5}$ | |
Fe sites	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.	Expt.	Calc.
$\%X,6c$	0	0.6	0	1.8	14.5(18)	23.8	19.3(18)	18.4	18.2(9)	18.4
$\%X,9d$	2.8(6)	1.4	0	0.7	0	0.3	0	1.2	0	1.0
$\%X,18f$	2.4(4)	2.1	1.4(11)	2.5	1.8(10)	0.2	1.2(10)	1.2	1.4(5)	1.2
$\%X,18h$	4.6(4)	5.4	7.0	4.9	1.7(10)	0	0.7(10)	0.4	0.8(5)	0.5

$Nd_2Fe_{17-\delta}X_\delta$ compounds were annealed the ratio of the site volumes remains constant, i.e., $V_{6c} > V_{18h} > V_{18f} > V_{9d}$. The atomic environment of an Fe site in Nd_2Fe_{17} is characterized by the number of Nd and Fe nearest neighbors. The $6c$ site has 13 Fe and 1 Nd, the $9d$ has 10 Fe and 2 Nd, the $18f$ has 10 Fe and 2 Nd, and the $18h$ has 9 Fe and 3 Nd.

The change of enthalpy of Nd_2Fe_{17} due to the substitution of an X atom for Fe in the x site can be written as

$$\Delta H^{tot}(x) = \Delta H_X^{tot}(x) - \Delta H_{Fe}^{tot}(x), \quad (1)$$

where $\Delta H_X^{tot}(x)$ and $\Delta H_{Fe}^{tot}(x)$ are the changes in the enthalpies due to the substitution of X and Fe in the x site, respectively, and can be written as

$$\Delta H_{X,Fe}^{tot}(x) = \Delta H_{X,Fe}^{sol}(x) + \Delta H_{X,Fe}^{el}(x) + \Delta H_{X,Fe}^{str}(x), \quad (2)$$

where $\Delta H_{X,Fe}^{sol}(x)$, $\Delta H_{X,Fe}^{el}(x)$ and $\Delta H_{X,Fe}^{str}(x)$ are contributions from the chemical, elastic, and structural effects, respectively, which we now discuss.

Chemical term

Since the value of δ is small ($\delta \leq 0.5$) it can be assumed that the X atoms are completely surrounded by Nd and Fe atoms in $Nd_2Fe_{16.5}X_{0.5}$ and that the enthalpies of solutions of solid A in solid B, ΔH_{A-B}^{sol} ($A, B = Nd, Fe, X$), appropriately describe the changes in enthalpy upon the addition of an X atom. A quantitative estimate of the difference between the chemical environments of the Fe sites in Nd_2Fe_{17} can be obtained following Miedema:[9]

$$\Delta H^{sol}(x) = \Delta H_{X-Nd}^{sol} S_{WS}^{Nd}(x) + \Delta H_{X-Fe}^{sol} S_{WS}^{Fe}(x)$$
$$- \Delta H_{Fe-Nd}^{sol} S_{WS}^{Nd}(x), \quad (3)$$

where the first two terms represent the change of enthalpy of solution due to the substitution of solid X in x site, $\Delta H_X^{sol}(x)$ and the third term is the change of enthalpy of solution due to the substitution of solid Fe in x site $\Delta H_{Fe}^{sol}(x)$.[10] $S_{WS}^{Nd}(x)$, and $S_{WS}^{Fe}(x)$ are the fractions of the Wigner-Seitz cell surfaces which an Fe atom in the site x shares with its Nd and Fe neighbors, respectively. The Wigner-Seitz cell surfaces are calculated from the atomic positions of Nd and Fe and the lattice constants of Nd_2Fe_{17} at 380 K. $S_{WS}^{Nd}(6c,9d,18f,18h) = 0.106$, 0.13, 0.211, 0.275 and

$S_{WS}^{Fe}(6c,9d,18f,18h) = 0.894$, 0.87, 0.789, 0.725, respectively. Because the experimental values for ΔH^{sol} for all X in Nd and X in Fe are not available, we have opted to use the semiempirical Miedema model to calculate the various solution enthalpies from Eq. (7) in Ref. 9:

$$\Delta H_{A-B}^{sol} = \frac{(V_A^{mol})^{2/3}}{(n_{ws}^{-1/3})_{av}} [-P(\Delta\phi^*)^2 + Q(\Delta n_{ws}^{1/3})^2 - R], \quad (4)$$

where A, $B = Nd$, Fe, X, V_A^{mol} is the molar volume of element A, P, and Q are empirically determined constants, $\Delta n_{ws}^{1/3} = (n_{ws}^A)^{1/3} - (n_{ws}^B)^{1/3}$ and $(n_{ws}^{-1/3})_{av} = \frac{1}{2}[(n_{ws}^A)^{-1/3} + (n_{ws}^B)^{-1/3}]$ where n_{ws}^A and n_{ws}^B are the electron densities of A and B, respectively. $\Delta\phi^* = \Delta\phi_A^* - \Delta\phi_B^*$ where ϕ_A^* and ϕ_B^* are the electronegativities of the pure metallic elements A and B, respectively. R is empirically determined and it is only present if ΔH_{A-B}^{sol} is being calculated for a transition and nontransition metal. The variation in most of the experimentally determined heats of solution is in the range of ± 10 kJ/mol.[17] This translates into an uncertainty of up to 15% in the calculated probabilities [Eq. (9)] for the most preferred Fe sites.

Elastic term

The quantitative estimate of the elastic energy due to the differences in the volume of the X or Fe atom and the volume of the x Fe site in Nd_2Fe_{17} can be calculated from Eshelby's[11] elastic continuum model:

$$\Delta H_{X,Fe}^{el}(x) = \frac{2K_{X,Fe}G_{Nd_2Fe_{17}}(V^c(x) - V_{X,Fe}^c)^2}{3K_{X,Fe}V^c(x) + 4G_{Nd_2Fe_{17}}V_{X,Fe}^c}, \quad (5)$$

where $K_{X,Fe}$ is the bulk modulus of X or Fe and $G_{Nd_2Fe_{17}}$ is the shear modulus of Nd_2Fe_{17} at the annealing temperature.[12] $V^c(x)$ and $V_{X,Fe}^c$ are the volumes of the x site and the atomic volumes of the X and Fe atoms, respectively, corrected for charge transfer and given by Eqs. (3), (3a), (6a/b) in Ref. 16:

$$V^c(x) = V(x) + \frac{V_{X,Fe}}{V_X^{mol}} \left[S_{WS}^{Nd}(x)\alpha_1(\phi_{Nd}^* - \phi_{X,Fe}^*) \frac{1}{n_{WS}^{Nd}} \right.$$

$$\left. + S_{WS}^{Fe}(x)\alpha_2(\phi_{Fe}^* - \phi_{X,Fe}^*) \frac{1}{n_{WS}^{Fe}} \right], \quad (6)$$

$$V_{X,Fe}^c = V_{X,Fe} + \frac{V_{X,Fe}}{V_X^{mol}} \left[S_{WS}^{Nd}(x)\alpha_1(\phi_{Nd}^* - \phi_{X,Fe}^*) \frac{1}{n_{WS}^{X,Fe}} \right.$$

$$\left. + S_{WS}^{Fe}(x)\alpha_2(\phi_{Fe}^* - \phi_{X,Fe}^*) \frac{1}{n_{WS}^{X,Fe}} \right], \quad (7)$$

where $\alpha_1 = -1.5(V_{X,Fe}^{mol})^{2/3}/[(n_{WS}^{Fe})^{-1/3} + (n_{WS}^{X,Fe})]^{-1/3}$ and $(V_{X,Fe}^{mol})^{2/3}/[(n_{WS}^{Nd})^{-1/3} + (n_{WS}^{X,Fe})]^{-1/3}$. $V(x)$, and $V_{X,Fe}$ are the volumes of the x site, and the atomic volumes of the X and Fe atoms, respectively. Eshelby derived Eq. (5) assuming that the volume of the site and the atoms are spherical. The average radii of each Fe site, $6c$, $9d$, $18f$, and $18h$, can be estimated from the Wigner-Seitz volume to surface ratio, $R(x) = 3V_{WZ}(x)/S_{WZ}(x)$, and is equal to 1.32, 1.26, 1.28, and 1.29 Å, respectively. If the uncertainties in the elastic constants[12] are of the order of 20%, the uncertainty in the calculated probabilities [Eq. (9)] for the most preferred Fe site is less than 5%. It is clear that the uncertainties in the elastic constants will not affect the calculated occupancies significantly.

Structural term

The structural ΔH^{str} contribution[18,19] reflects the preference for d-electron metals to crystallize in one of the main crystallographic structures, bcc, fcc, and hcp, depending on the number of valence electrons per atom z. Niessen *et al.*[16] assumed that ΔH^{str} varies systematically with the average number of valence electrons per atom in solid solutions of transition metals as long as the two metals form a common band of d-type electron states. Dissolving metal X in matrix M changes the enthalpy that stabilizes the crystal structure of the matrix element. The average number of valence electrons per atom is a locally defined quantity being determined by the solute atom and its nearest neighbors. Therefore, in Nd_2Fe_{17}, the difference in the local environment of each site will cause a difference in the average number of valence electrons of each x site, $z(x)$. Here, we assume that Nd behaves like Y and La, i.e., $z = 3$.[20] The change in the enthalpy due to the substitution of X or Fe in the x site, $\Delta H_{X,Fe}^{str}(x)$, can be written following Eq. 9 in Ref. 17 as

$$\Delta H_{X,Fe}^{str}(x) = [z_{X,Fe} - z_M(x)] \frac{dE_{\sigma(M)}(z_M(x))}{dz_M(x)} + E_{\sigma(M)}(z_M(x))$$

$$- E_{\sigma(X,Fe)}(z_{X,Fe}), \quad (8)$$

where $z_{X,Fe}$ is the number of valence electrons per X or Fe atom and $z_M(x)$ is the average number of valence electrons of the nearest-neighbor atoms surrounding the x site. $\sigma(M)$ and $\sigma(X,Fe)$ indicate the crystal structure of Nd_2Fe_{17}, and for the elements X and Fe, respectively. The values for $E_{\sigma(X,Fe)}(z_{X,Fe})$ are taken from Table I, Ref. 17. From Fig. 2, Ref. 17, we see that $E_\sigma(z)$ behaves similarly for closed-packed structures, fcc and hcp, as opposed to $E_\sigma(z)$ for bcc. For R_2Fe_{17} (R light rare-earth), the rhombohedral structure is a closed-packed structure and is similar to hcp. Therefore,
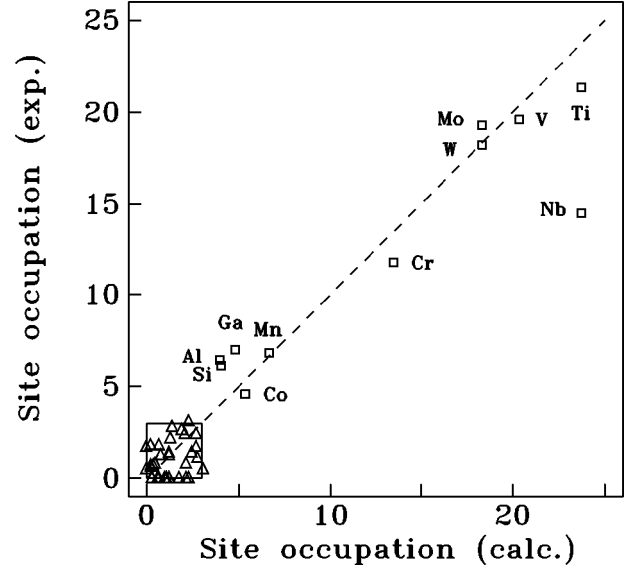

FIG. 1. Calculated versus experimental fractional site occupations of the X atoms in all x Fe sites in Nd_2Fe_{17}. The unfilled squares and triangles denote the fractional site occupations versus experimentally determined site preferences and avoidances, respectively.

we take $\sigma(M)$ to be hcp.[20] As the samples were annealed at 1300 K, we take Ti, Mn, Fe, and Co to have the β-Ti, β-Mn, γ-Fe, and α-Co structures, respectively. We assume a continuous variation of $E_\sigma(z)$ as a function of z in Fig. 2, Ref. 17. Then $dE_{\sigma(M)}(z_M(x))/dz_M(x)$ and $E_{\sigma(M)}(z_M(x))$ were calculated from a spline function used to obtain a smooth curve connecting the points presented in Fig. 2, Ref. 16. For nontransition metals X, $\Delta H_X^{str}(x) = 0$.

Since the change of volume upon substitution of an X atom for Fe is small we can take $p\Delta V \approx 0$. Then, the change of binding energy due to this substitution, $\Delta E(x)$, can be represented by $\Delta H^{tot}(x)$. The probability for an X atom substituting for Fe in the site x can be simply given by

$$P(x) = \frac{g(x)e^{-\Delta H^{tot}(x)/kT}}{\sum_x g(x)e^{-\Delta H^{tot}(x)/kT}}, \quad (9)$$

where $g(x)$ is the number of the x sites in formula unit, k is the Boltzmann constant and T is taken to be 1300 K, the temperature at which the $Nd_2Fe_{16.5}X_{0.5}$ compounds were annealed. In calculating $P(x)$, we assume that each formula unit of Nd_2Fe_{17} has a maximum of one X atom, and that the X atoms are uniformly distributed throughout the sample. The uniform distribution of the X atoms in the sample is expected because of the non-negative ΔH_{X-Fe}^{sol} and a large configurational entropy at the temperature of annealing.

The occupation probabilities calculated from Eq. (9) are presented along with the experimentally determined site occupations in $Nd_2Fe_{16.5}X_{0.5}$, Table I and Fig. 1. The results show that the model precisely determines which sites are preferentially occupied by the X atoms; calculated values are within 35% of the experimental values for all X elements. Moreover, the model correctly predicts which sites are avoided by the X elements. It is important to stress that all three terms $\Delta H_{X,Fe}^{sol}$, $\Delta H_{X,Fe}^{el}$, and $\Delta H_{X,Fe}^{str}$ have to be taken into account in order to correctly explain the experimentally

observed substitutions. If the model considers only $\Delta H^{\text{sol}}_{X,\text{Fe}}$, the preferential occupations of all transition X elements, except Co, in the $6c$ and $9d$ sites are obtained. This is obviously not correct since the experimental results show complete avoidance of the $9d$ site by all X elements except Mn and Co. The occupation of the $9d$ site is governed by $\Delta H^{\text{el}}_{X,\text{Fe}}$. The occupation probabilities calculated if both $\Delta H^{\text{sol}}_{X,\text{Fe}}$ and $\Delta H^{\text{el}}_{X,\text{Fe}}$ are present, correctly predict the sites preferentially occupied by the X elements. However, for transition metals the occupations are significantly underesti-

mated: up to 50%. In Nd_2Fe_{17}, due to the difference in the valences between Nd and Fe ($z_{\text{Nd}}=3$ and $z_{\text{Fe}}=8$), $z_M(x)$ differs significantly. This is reflected in the large contribution of $\Delta H^{\text{str}}_{X,\text{Fe}}$ to $P(x)$. In conclusion, a *quantitative* account of Fe substitutions for both *nontransition* and *transition* atoms in Nd_2Fe_{17} can be understood by considering a model which includes contributions from the chemical, elastic, and structural terms. The model is general in scope and can be applied to any intermetallic compound where the site occupations of elemental substitutions need to be determined.

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found by an extrapolation from the lower temperature values (Refs. 13, 14). If one assumes that the Curie temperature T_C changes linearly with volume in Nd_2Fe_{17}, the bulk modulus of Nd_2Fe_{17}, $K_{Nd_2Fe_{17}}$, can be found from the value of dT_c/dP reported by Isnard (Ref. 15). This value for $K_{Nd_2Fe_{17}}$ is comparable to the bulk modulus of α-Fe at room temperature. Hence, we will assume that the value of the shear modulus of α-Fe, at the annealing temperature, appropriately represents that of $G_{Nd_2Fe_{17}}$.

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