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Structure, magnetic properties, and magnetovolume effect of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$

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Abstract

A novel compound $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ was synthesized. The structure and magnetic properties of the compound were investigated by means of x-ray powder diffraction (XRD) analysis and magnetic measurements. $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ crystallizes in a monoclinic $\text{Nd}_3(\text{Fe}, \text{Ti})_{29}$ structure with space group $A2/m$. The lattice constants of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ are $a = 10.6131(1) \text{ \AA}$, $b = 8.5897(1) \text{ \AA}$, $c = 9.7518(1) \text{ \AA}$, and $\beta = 96.69(4)^\circ$, respectively. Rietveld refinement of the XRD data reveals that the Re atoms have a strong preference to occupy the three dumb-bell 4g, 4i3, and 4i4 sites. The preferential occupancy of the Re is predominantly determined by the atomic size effect. The final refined stoichiometry $\text{Nd}_3\text{Fe}_{26.65}\text{Re}_{2.35}$ is in good agreement with the result of chemical analysis: $\text{Nd}_3\text{Fe}_{26.6(1)}\text{Re}_{2.39(3)}$. $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ is found to be of planar anisotropy perpendicular to the [204] direction at room temperature. The Curie temperature T_C , saturation magnetization M_S , and magnetocrystalline anisotropy field H_A are 354 K, $52.9 \mu_B/\text{f.u.}$, and 20.6 T, respectively. The relatively low T_C is related to the preferential occupations of the Re of the 4g, 4i3, and 4i4 sites. The temperature-dependent XRD experiment shows a contraction of the unit-cell volume with temperature around T_C , which can be ascribed to the vanishing magnetism. The magnetism has a significant effect on the lattice parameters a , b , c , and β , which is anisotropic in character.

1. Introduction

Investigation of Fe-rich rare-earth intermetallic compounds as permanent magnet materials has been extensive in recent years [1–3]. Early interest was focused predominantly on the $\text{R}(\text{Fe}, \text{M})_{12}$ compounds crystallizing in the tetragonal ThMn_{12} structure with space group $I4/mmm$ where R represents a rare earth and M a third element. Because the binary RFe_{12} compound does not exist, introduction of the third element, $\text{M} = \text{Ti}, \text{V}, \text{Cr}, \text{Mo}, \text{Nb}, \text{W}, \text{Si}, \text{Al}$, etc, is indispensable for stabilizing $\text{R}(\text{Fe}, \text{M})_{12}$ compounds [4–8]. Likewise, the $\text{R}_3(\text{Fe}, \text{M})_{29}$

compounds with monoclinic structure discovered a decade ago cannot be formed unless a stabilizing element, $M = \text{Ti, V, Cr, Mo, Nb, Ta, W, etc.}$, is added [9–19]. The elements stabilizing the 1:12 structure, such as Ti, V, Cr, Mo, and Nb, usually have positive solution enthalpies in the rare earths except for Si and Al. In contrast, almost all elements capable of stabilizing the 3:29 structure appear to have a positive solution enthalpy in the rare earths and a larger atomic radius than that of Fe. It has been established that the third element not only plays an important role in the formation of the 1:12 and 3:29 structures, but also exerts a strong influence on the magnetic properties of these compounds.

Re has a larger atomic radius than that of Fe but a negative solution enthalpy in the rare earths (La excluded). Therefore it would be interesting to examine the possibility of the formation of $\text{R}_3(\text{Fe, Re})_{29}$ compounds. In this contribution we report the synthesis, crystal structure, magnetic properties, and temperature dependence of the lattice parameters of a novel compound $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$. Due to a large scattering contrast between Re and Fe, the preferential occupancies of Re and Fe of different crystallographic sites in the $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ structure can be unambiguously determined by Rietveld refinement of x-ray powder diffraction (XRD) data.

2. Experimental procedure

Samples of $\text{Nd}_3\text{Fe}_{29-x}\text{Re}_x$ with $x = 1.8, 2.0, 2.4, 2.5, 2.6, 2.8,$ and 3.0 were prepared by arc melting of the constituting elements Nd, Fe, and Re with purity better than 99.9% in a water-cooled copper hearth under a high-purity argon atmosphere. An appropriate excess amount of Nd was added to compensate for the weight loss during arc melting and subsequent high-temperature annealing. The ingots were melted several times to ensure homogeneity. The samples thus obtained were sealed in an evacuated quartz tube and homogenized at 1373 K for one week; this was followed by water quenching.

XRD experiments were performed on a Rigaku D/max 2500 diffractometer with $\text{Cu K}\alpha$ radiation ($40 \text{ kV} \times 200 \text{ mA}$) and a graphite monochromator. A step scan mode was adopted with a step width of $2\theta = 0.02^\circ$ and a sampling time of 1 s. Magnetization versus temperature curves were measured by using a vibrating-sample magnetometer (VSM). The field dependence of the magnetization was measured by a superconducting quantum interference device (SQUID) magnetometer. An XRD experiment on a magnetically aligned sample was employed to determine the easy magnetization direction (EMD) at room temperature.

3. Results and discussion

3.1. Crystal structure

Phase identification of the samples of $\text{Nd}_3\text{Fe}_{29-x}\text{Re}_x$ with different x -values was performed by means of XRD analysis. The samples with $x < 2.0$ are composed of the 2:17 major phase and a small amount of the 3:29 phase and α -Fe, while the sample with $x = 3.0$ consists of the 2:17 phase and a small amount of the 3:29 phase under our experimental conditions. The samples with $x = 2.4$ and 2.6 consist of the 3:29 major phase and the minor 2:17 phase and α -Fe as impurities, whereas the sample with $x = 2.5$ is almost single phase with only a little α -Fe as an impurity, as shown in figure 1. In addition, no noticeable relative position shifts of the XRD peaks of the samples with $x = 2.4, 2.5,$ and 2.6 were detected, suggesting that the solid-solution regime of Re in $\text{Nd}_3\text{Fe}_{29-x}\text{Re}_x$ is very narrow.

We adopted the monoclinic $\text{Nd}_3(\text{Fe, Ti})_{29}$ structure with space group $A2/m$ [20] as the initial structure for performing the Rietveld refinement of the XRD data of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ using the program DBW-9411 [21, 22]. The refinement results are illustrated in figure 2 and

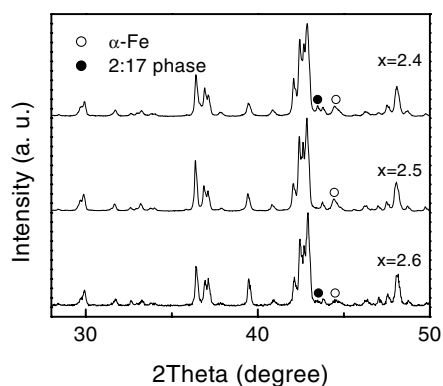


Figure 1. XRD patterns of Nd₃Fe_{29-x}Re_x with different x -values.

Table 1. Rietveld refinement results for the Nd₃Fe_{26.5}Re_{2.5} compound with space group $A2/m$, occupancies of the Re atom, average distances (AD) of sites to neighbouring Fe and Nd, and the numbers of neighbouring atoms.

Atoms	Sites	x	y	z	AD of sites to neighbouring Fe, Nd (Å)		Re (%) occupancy	The number of neighbouring atoms
Nd	2a	0.0	0.0	0.0	3.1544			20Fe
Nd	4i	0.4029(1)	0.0	0.8142(1)	3.1622			19Fe
Fe/Re	2c	0.5	0.0	0.5	2.5032	3.3450	2.87	10Fe + 2Nd
Fe/Re	4e	0.0	0.25	0.25	2.5166	3.2486	2.28	10Fe + 2Nd
Fe/Re	4g	0.0	0.3588(1)	0.0	2.6974	3.0845	39.33	13Fe + 1Nd
Fe/Re	4i1	0.1099(2)	0.0	0.7224(2)	2.5717	3.1052	0.55	10Fe + 2Nd
Fe/Re	4i2	0.2941(3)	0.0	0.0957(1)	2.5796	3.1594	1.43	9Fe + 3Nd
Fe/Re	4i3	0.2529(2)	0.0	0.5232(2)	2.6936	3.0907	28.69	13Fe + 1Nd
Fe/Re	4i4	0.1397(4)	0.0	0.2953(2)	2.6976	3.0757	27.67	13Fe + 1Nd
Fe/Re	8j1	0.6250(2)	0.1434(1)	0.6853(3)	2.5880	3.0665	1.91	10Fe + 2Nd
Fe/Re	8j2	0.8039(3)	0.2195(2)	0.0895(3)	2.5899	3.0679	2.66	10Fe + 2Nd
Fe/Re	8j3	0.4051(2)	0.2502(1)	0.0657(4)	2.5606	3.1969	2.11	9Fe + 3Nd
Fe/Re	8j4	0.2004(1)	0.2566(4)	0.1572(1)	2.5040	3.2816	1.41	10Fe + 2Nd

$a = 10.6131(1)$, $b = 8.5897(1)$, $c = 9.7518(1)$ Å, $\beta = 96.69(4)^\circ$, $V = 882.9(4)$ Å³
 $R_p = 7.55\%$, $R_{wp} = 9.64\%$, $R_{exp} = 5.31\%$

table 1. The pattern factor R_p , the weighted pattern factor R_{wp} , and the expected pattern factor R_{exp} are 7.55, 9.64, and 5.31%, respectively. The lattice parameters of Nd₃Fe_{26.5}Re_{2.5} are $a = 10.6131(1)$ Å, $b = 8.5897(1)$ Å, $c = 9.7518(1)$ Å, and $\beta = 96.69(4)^\circ$.

Due to the large scattering contrast between Fe and Re, the preferential occupancies of the Re atoms of different crystallographic positions in the Nd₃Fe_{26.5}Re_{2.5} structure are expected to be determined unambiguously by means of the Rietveld refinement. Upon performing the refinement, we purposely put the Re atoms on all the possible Fe sites in the Nd₃Fe_{26.5}Re_{2.5} structure and then refined the occupancies as free parameters. The results indicated that 81.39% of the Re atoms occupy preferentially the three dumb-bell sites 4g, 4i3, and 4i4, while the remaining 18.61% are distributed over the other Fe sites, as outlined in table 1.

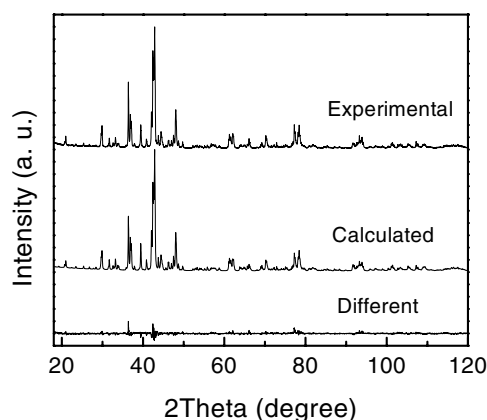


Figure 2. Experimental and calculated XRD patterns of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$, and the difference between them.

According to the Miedema model [23], the solution enthalpies of Re and Fe in Nd are worked out to be -7 and 2 kJ mol^{-1} , respectively. From the viewpoint of enthalpy, it would be energetically favourable for the Re atoms to preferentially occupy the sites that have the shortest distance to and the largest nearest-neighbour number of Nd atoms and thus the largest contact area with Nd, such as the 4i2, 8j3 sites and the like. Such a prediction is, however, inconsistent with the Rietveld refinement results. Hence, some other factors should be taken into consideration to give a reasonable explanation of the site preference of the Re atoms. The structural parameters given by the Rietveld refinement allows us to calculate the average distances of the Fe sites to their nearest-neighbour Fe sites, which are listed in table 1. For the 4g, 4i3, and 4i4 sites the average distances are 2.6974, 2.6936, and 2.6976 Å, respectively, the longest among all Fe sites. Assuming that the Re and Fe atoms behave as hard spheres with the metallic radii of 1.38 and 1.27 Å, respectively, one can conclude that the 4g, 4i3, and 4i4 sites have enough space to accommodate the Re atoms. In contrast, the average distances of other Fe sites are shorter than 2.60 Å. If these sites are occupied by the Re atoms, relatively large distortions will be produced, which is energetically unfavourable. Therefore, the enthalpy and atomic size effects play opposite roles in governing the preferential occupations of the Re atoms. The preferential occupation of the majority of the Re atoms of the 4g, 4i3, and 4i4 sites can be readily understood in terms of the dominating role of atomic size compared to enthalpy. A similar explanation was applied for the compound $\text{Gd}_3\text{Fe}_{28}\text{Re}$ [24].

The Rietveld refinement result suggests that the Re atoms occupy all the Fe sites in $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$. The occupancy of the Re atoms of the non-dumb-bell Fe sites ranges from 0.55 to 2.87%. Such a small value of occupancy might be attributed to an uncertainty of the refinement results, leading to a case like that for $\text{Nd}_3\text{Fe}_{27.76}\text{Ti}_{1.24}$ reported in [20], i.e. the Re atoms occupy exclusively the three dumb-bell Fe sites. Nevertheless, the possibility of the Re atoms occupying the non-dumb-bell Fe sites should not be excluded, since the metallic radius of the Re atom is smaller than that of the Ti atom and the Re content in $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ is larger than the Ti content in $\text{Nd}_3\text{Fe}_{27.76}\text{Ti}_{1.24}$. Usually, the smaller the third element M, the more likely it is that the M will occupy the non-dumb-bell Fe sites and that there will be a larger content of M in $\text{R}_3\text{Fe}_{29-x}\text{M}_x$ [25]. In the compounds $\text{Nd}_3\text{Fe}_{23.52}\text{Cr}_{5.38}$ and $\text{Nd}_3\text{Fe}_{17.8}\text{Mn}_{11.2}$, the occupancy of the Cr atoms of the non-dumb-bell Fe sites ranges from 5.1 to 20.4% (the 2c, 4i2, and 8j3 sites are not occupied by the Cr atoms) and that of the Mn atoms from 2.6 to 40.4% (all the Fe sites are partially occupied by Mn atoms) [20]. If we simply scale the

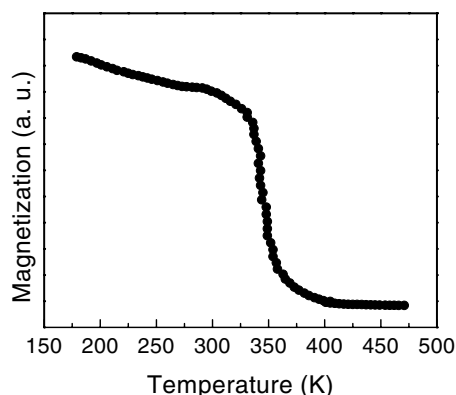


Figure 3. The temperature dependence of the magnetization of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ in an applied magnetic field of 0.05 T.

occupancy by the Cr or Mn contents, the above-mentioned occupancy would be 2.2–8.7 or 0.5–8.5% for the Cr or Mn contents corresponding to the Re content in $\text{Nd}_3\text{Fe}_{26.65}\text{Re}_{2.35}$ (for the refined stoichiometry, see below). In addition, the negative enthalpy of solution of the Re in Nd also favours a partial occupation of the non-dumb-bell Fe sites by the Re atoms.

On the basis of the Rietveld refinement results, the stoichiometry is found to be $\text{Nd}_3\text{Fe}_{26.65}\text{Re}_{2.35}$, which deviates slightly from the nominal stoichiometry $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$. Chemical analysis of the sample by inductively coupled plasma atomic emission spectroscopy (ICP-AES, TJACo) gave the stoichiometry $\text{Nd}_3\text{Fe}_{26.6(1)}\text{Re}_{2.39(3)}$, which is in good accordance with our refinement result. In the following discussion, the nominal stoichiometry of the compound, i.e. $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$, is referred to.

3.2. Magnetic properties

Figure 3 shows the temperature dependence of the magnetization of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ in a magnetic field of 0.05 T. The Curie temperature, $T_C = 354$ K, was derived by extrapolating M^2 to zero on the M^2 – T curve. To determine the EMD at ambient temperature and the magnetocrystalline anisotropy field (H_A), magnetically aligned samples were employed. Fine powder (<20 μm) and epoxy resin at a weight ratio of 1:1 were mixed and filled into disc- and column-like containers, respectively. The disc- and column-like containers rotated in a magnetic field of 1 T perpendicular to their axes until the mixture hardened. The disc- and column-like samples obtained in this way were used for the determination of the EMD by XRD and H_A by magnetization measurement, respectively. The XRD pattern of the magnetically aligned sample is shown in figure 4. It is evident that the peak (204) is much intensified while the other peaks are severely weakened. As is known, the 3:29 structure is a derivative of the fundamental CaCu_5 structure. In terms of the matrix transformation relations, the (204) peak in the 3:29 structure corresponds to the (002) peak in the CaCu_5 structure. Thus it can be readily inferred that the EMD of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ at room temperature is an easy plane direction (noting that the aligning field was applied parallel to the plane of the disc-like sample for the XRD experiment).

Figure 5 plots the magnetization versus field curves (M – H) of the free fine powder and magnetically aligned samples of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ at 5 K. By extrapolating $1/H$ to zero on the M – $1/H$ curve of the sample for free fine powder, the total magnetization of 135.9 $\text{A m}^2 \text{kg}^{-1}$, was derived. According to the refinement result, the weight fraction of α -Fe is about 4.8%.

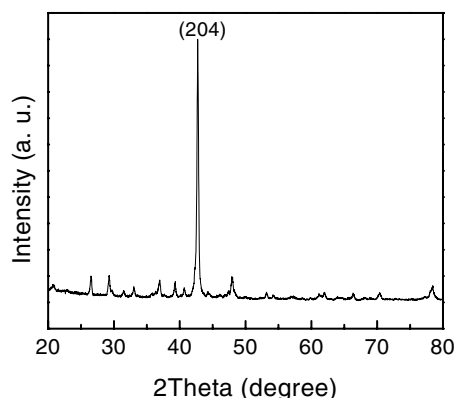


Figure 4. The XRD pattern of the magnetically aligned sample of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ at room temperature.

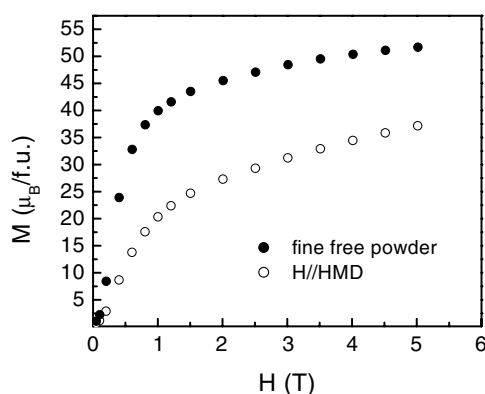


Figure 5. Field dependences of the magnetization of the free fine powder and magnetically aligned samples of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ at 5 K. 'H//HMD' means that the applied field during the magnetization measurement is along the HMD, i.e. parallel to the axis of the column-like sample in our case.

It is well known that the saturation magnetization value of $\alpha\text{-Fe}$ is $221.7 \text{ A m}^2 \text{ kg}^{-1}$ at 4.2 K. The contribution of $\alpha\text{-Fe}$ to the total magnetization was subtracted to derive the saturation magnetization of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$, $M_S = 125.3 \text{ A m}^2 \text{ kg}^{-1}$ ($52.9 \mu_B/\text{f.u.}$). Assuming that the moment of Nd^{3+} is $3 \mu_B$, we can work out the average moment of Fe, $\langle \mu_{\text{Fe}} \rangle = 1.65 \mu_B$. In addition, we can also obtain the anisotropy field of $H_A = 20.6 \text{ T}$ at 5 K from figure 5 by linearly extrapolating ΔM to zero on the $\Delta M-H$ curve ($\Delta M = M_{\parallel} - M_{\perp}$), where M_{\parallel} is taken as that of the free fine powder and M_{\perp} as the magnetization of the magnetically aligned sample with an applied field along the hard magnetization direction (HMD). However, one should treat this derived H_A -value with caution, since both figures 4 and 5 reveal that the magnetic particles were not perfectly aligned at room temperature under a field of 1 T, which would give rise to an overestimated value of H_A from the extrapolation method used in this work.

In comparison to other isostructural compounds $\text{Nd}_3\text{Fe}_{29-x}\text{M}_x$ ($M = \text{V}, \text{Cr}, \text{and Ti}$) [26, 27], $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ exhibits a comparable saturation magnetization but a relatively low Curie temperature (see table 2). In the $\text{R}_3(\text{Fe}, \text{M})_{29}$ structure the Fe-Fe bond length usually spans in an interval from 2.3 to 3.0 Å. The Fe moments with short bonds are antiferromagnetically coupled while those with long bonds are ferromagnetically coupled. The couplings of the Fe moments at the dumb-bell 4g, 4i3, and 4i4 sites with the neighbouring

Table 2. The unit-cell volume V , Curie temperature T_C , saturation magnetization M_S , and average moment of Fe (μ_{Fe}) for Nd₃Fe_{29-x}M_x (M = V, Cr, Ti, and Re) compounds.

Compounds	V (Å ³)	T_C (K)	M_S (4.2 K)	
			(μ_B /f.u.)	(μ_B)
Nd ₃ Fe _{27.0} V _{2.0} [26]	882.6	455	54.7	1.69
Nd ₃ Fe _{24.5} Cr _{4.5} [27]	875.9	413	49.9	1.67
Nd ₃ Fe _{27.85} Ti _{1.15} [27]	884.5	396	58.2 ^b	1.77 ^b
Nd ₃ Fe _{26.5} Re _{2.5}	882.9	354	52.9 ^a	1.65 ^a

^a 5 K measurement.^b 12 K measurement.

Fe moments are mainly ferromagnetic, and have the maximum average bond lengths shown in table 1. The bond-length variation due to the replacement of the Fe at the dumb-bell sites by a small amount of M with larger atomic radius will not have a significant effect on the Curie temperature. For the compound Nd₃Fe_{24.5}Cr_{4.5} a substantial proportion of the Cr atoms occupy non-dumb-bell sites [20], increasing the Fe–Fe distance and weakening the antiferromagnetic coupling, and consequently the compound exhibits a higher Curie temperature than Nd₃Fe_{27.85}Ti_{1.15} and Nd₃Fe_{26.5}Re_{2.5}, since both the Ti in Nd₃Fe_{27.85}Ti_{1.15} [20] and the Re in Nd₃Fe_{26.5}Re_{2.5} strongly prefer the dumb-bell sites. The T_C of Nd₃Fe_{26.5}Re_{2.5} being lower than that of Nd₃Fe_{27.85}Ti_{1.15} can be attributed to a higher Re concentration in the former. For the compound Nd₃Fe₂₇V_{2.0}, the low V content and a possible occupation of the V atoms of the non-dumb-bell Fe sites may be partially responsible for it having the highest T_C among the compounds listed in table 2. Since the metallic radius of the V atom is smaller than those of Ti and Re, the V atoms are more likely to occupy the smaller non-dumb-bell Fe sites than the Ti and Re atoms. Unfortunately, the occupation of the V atoms in R₃Fe_{29-x}V_x has not yet been well characterized, due to the facts that its neutron scattering factor is close to zero and its x-ray scattering factor is close to that of Fe [25].

3.3. Temperature dependences of the lattice parameters

The XRD data for Nd₃Fe_{26.5}Re_{2.5} were collected at various temperatures by using a step scan mode and were Rietveld refined to obtain accurate lattice constants. The lattice parameters as a function of temperature are shown in figure 6. Anomalies of the lattice parameters around T_C are observed. A similar feature was reported for other rare-earth–transition metal compounds [28–31]. Figure 6 shows that the unit-cell volume increases at a rate of 0.0042 Å³ K⁻¹ from 77 to 300 K, and then decreases at 0.0035 Å³ K⁻¹ from 300 K to T_C , and finally increases at 0.031 Å³ K⁻¹ above T_C . The lattice parameters a and b vary with temperature similarly to the unit-cell volume. The lattice parameter c initially decreases with increasing temperature below 300 K, and then levels off between 300 K and T_C , and again increases above T_C . The angle β increases at a relatively high rate from 77 K to T_C and then increases at a much lower rate.

In the temperature interval of 300 K to T_C the unit-cell volume contracts with temperature, which is considered to be associated with the magnetovolume effect [32]. The rate of the volume increase below 300 K is about an order of magnitude smaller than that above T_C , suggesting that the magnetism plays a dominant role. The temperature dependences of a , b , and c indicate that the effects of the magnetism on a , b , and c are of anisotropic nature. The magnetism leads the lattice parameters a and b to have a similar variation tendency but causes c to decrease with increasing temperature. The variation of the angle β with temperature below T_C is also strongly enhanced by the presence of the magnetism, implying that the distribution of charge might be changed.

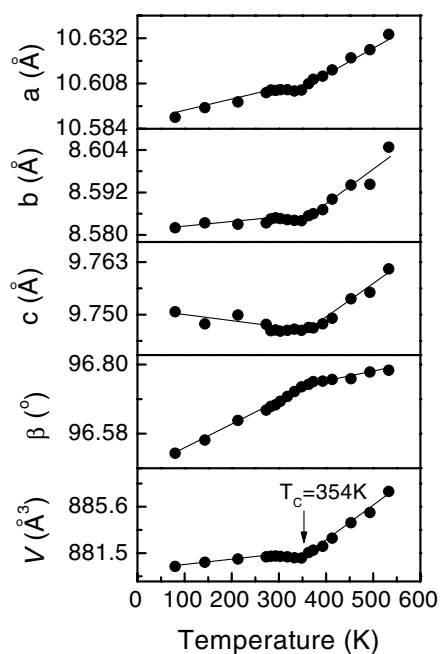


Figure 6. Temperature dependences of the lattice parameters a , b , c , β , and V of $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$; the curves are guides to the eye.

4. Conclusions

The Re atom, which has a negative solution enthalpy with Nd, can be used to stabilize the compound $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ crystallizing in the monoclinic structure with space group $A2/m$. Rietveld refinements of the XRD data revealed that the Re atoms strongly prefer the three dumb-bell 4g, 4i3, and 4i4 sites. The preferential occupancy of the Fe sites by the Re atoms may be ascribed to a competition of the atomic size and enthalpy effects, whereas the atomic size plays a crucial role. The final refined stoichiometry is $\text{Nd}_3\text{Fe}_{26.65}\text{Re}_{2.35}$, in good agreement with $\text{Nd}_3\text{Fe}_{26.6(1)}\text{Re}_{2.39(3)}$ derived from the chemical composition analysis. It is derived that $\text{Nd}_3\text{Fe}_{26.5}\text{Re}_{2.5}$ has a planar anisotropy perpendicular to the [204] direction at room temperature. The Curie temperature T_C , saturation magnetization M_S , and anisotropy field H_A are 354 K, $52.9 \mu_B/\text{f.u.}$, and 20.6 T, respectively. The relatively low T_C is supposed to be associated with the preferential occupations of the Re atoms of the 4g, 4i3, and 4i4 sites. The temperature-dependent XRD experiments indicated that the contraction of the cell volume with increasing temperature occurred around the Curie temperature, which is related to the magnetovolume effect. The effects of the magnetism on the lattice parameters a , b , and c are, remarkably, of anisotropic nature.

Acknowledgments

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References

- [1] de Mooij D B and Buschow K H J 1988 *J. Less-Common Met.* **136** 207
- [2] Buschow K H J, de Mooij D B, Brouha M, Smit H H A and Thiel R C 1988 *IEEE Trans. Magn.* **24** 1611
- [3] Jurczyk M and Christjakov O D 1989 *J. Magn. Magn. Mater.* **82** 239
- [4] Sun H, Akayama M, Tatami K and Fuji H 1993 *Physica B* **183** 33
- [5] Kuz'min M D 2000 *J. Appl. Phys.* **88** 7217
- [6] Buschow K H J 1988 *J. Appl. Phys.* **63** 3130
- [7] del Moral A, Algarabel P A, Marquina C, de la Fuente C and Ibarra M R 1994 *J. Magn. Magn. Mater.* **131** 247
- [8] Vert R, Fruchart D, Landa B G, Gignoux D and Amako Y 1998 *J. Alloys Compounds* **275–77** 611
- [9] Hu Z and Yelon W B 1994 *J. Appl. Phys.* **76** 6147
- [10] Fuerst C D, Pinkerton F E and Herbst J F 1994 *J. Magn. Magn. Mater.* **129** L115
- [11] Ryan D H and Cadogan J M 1994 *J. Appl. Phys.* **76** 6150
- [12] Han X F, Pan H G, Liu H L and Yang F M 1997 *Phys. Rev. B* **56** 8867
- [13] Shcherbakova Y V, Ivanova G V, Makarova G M, Belozеров Y V and Ermolenko A S 1995 *J. Magn. Magn. Mater.* **140** 1099
- [14] Yang F M, Nasunjilegal B, Wang J L, Pan H Y, Qing W D and Zhao R W 1994 *J. Appl. Phys.* **76** 1971
- [15] Huang F, Liang J K, Liu Q L, Chen X L and Hou G Y 1999 *J. Appl. Phys.* **85** 6686
- [16] Yang D, Wang J L, Tang N, Shen Y P and Yang F M 1999 *Appl. Phys. Lett.* **74** 4020
- [17] Liu Q L, Rao G H, Liang J K and Shen B G 2000 *J. Appl. Phys.* **88** 4241
- [18] Huang F, Liang J K, Chen X L and Chen Y 1999 *J. Alloys Compounds* **291** 239
- [19] Liu Q L, Rao G H and Liang J K 2000 *J. Phys.: Condens. Matter* **12** 5473
- [20] Yelon W B and Hu Z 1996 *J. Appl. Phys.* **79** 1330
- [21] Rietveld H M 1967 *Acta Crystallogr.* **229** 151
- [22] Young R Y, Sakthirel A, Moss T S and Paiva-Santos C O 1995 *J. Appl. Crystallogr.* **28** 366
- [23] Miedema A R, de Chatel P F and de Boer F R 1980 *Physica B+C* **100** 1
- [24] Chu W G, Rao G H, Yang H F, Liu G Y and Liang J K 2001 *J. Phys.: Condens. Matter* **13** L441
- [25] Liang J K, Liu Q L, Huang F, Rao G H and Chen X L 2002 *Prog. Natural Sci.* **12** 81
- [26] Han X F, Yang F M and Miyazaki T 1998 *J. Magn. Soc. Japan* **22** 351
- [27] Cadogan J M, Li H S, Margarian A, Dunlop J B, Ryan D H, Collocott S J and Davis R L 1994 *J. Appl. Phys.* **76** 6138
- [28] Gratz E *et al* 1995 *J. Phys.: Condens. Matter* **7** 597
- [29] Meisner G P and Fuerst C D 1986 *IEEE Trans. Magn.* **22** 744
- [30] Givord D and Lemaire R 1974 *IEEE Trans. Magn.* **10** 109
- [31] Kamarád J, Arnold Z, Morellon L, Algarabel P A, Ibarra M R and Fuerst C D 1996 *J. Appl. Phys.* **79** 4656
- [32] Rancourt D G and Zhang M D 1996 *Phys. Rev. B* **54** 12 225