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The magnetic structures of $NdCu_2$ in zero field

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Abstract. The magnetic structure of $NdCu_2$ has been investigated by means of neutron diffraction as a function of temperature between 1.4 K and 8 K in zero external field. The diffraction patterns were obtained on the multidetector DN5 at the SILOE reactor of CENG. Two magnetic phases were observed between 1.4 K and $T_N = 6.5$ K. In both phases the magnetic structure can be described by an oscillating component of the Nd moments, which are oriented along the b-direction. In the high-temperature phase between 5.2 K and T_N a sinusoidal oscillating component with wavevector $\tau^* = (0.62, 0.042, 0)$ is obtained. Accordingly, the magnetic structure is incommensurate with the lattice. Below 4 K the structure becomes commensurate with the lattice and the wavevector is given by $\tau = (0.6, 0, 0)$. This means that in the low-temperature phase the structure is exactly a transversely oscillating component. Additionally a progressive squaring up from the appearance of the third harmonic 3τ in the range from 4.0 K down to 1.4 K is observed. At 1.4 K the amplitudes of the fundamental and the third harmonic oscillation are $2.32\mu_B$ and $0.9\mu_B$, respectively. The ratio of these two values agrees with that expected for complete squaring up. Around 4.4 K the spectra seem to be determined by a superposition of the high- and low-temperature phases.

1. Introduction

Among the RM_2 compounds (R = rare earth, M = transition metal) the $MgCu_2$ type structure (space group $Fd3m$) exists for all 3d metals from Mn to Ni. However, the 1:2 compounds with Cu exhibit (with the exception of $LaCu_2$) the orthorhombic $CeCu_2$ type structure with the space group $Imma$. $LaCu_2$ displays the hexagonal AlB_2 structure [1]. In this connection it is of interest to note that the RNi_2 compounds show structural instabilities around 700–900 K. This high-temperature phase can be considered as a predecessor of the orthorhombic $CeCu_2$ structure in the following RCu_2 series [2]. Our preliminary investigations of the temperature variation of the lattice parameters by x-ray diffraction, which were performed for nearly all of the RCu_2 compounds (except $EuCu_2$), revealed that the $CeCu_2$ type structure exists for all compounds down to 4.2 K [2]. Initial magnetic investigations on RCu_2 have been performed by Sherwood *et al* for all lanthanides [3]. They observed metamagnetic behaviour, from which they deduced that these compounds order antiferromagnetically (AF). This was first confirmed by neutron diffraction measurements by Brun *et al* , who interpreted their results in terms of collinear antiferromagnetism at 4.2 K with spins directed along the a-direction [4]. After considering the stability conditions Brun *et al* conclude on the grounds of molecular field calculations that the deduced structure at 4.2 K in $TbCu_2$ is not the most stable as far as exchange interactions are concerned. Other non-collinear or spiral AF structures have lower energy. Thus the observed collinearity must result from strong anisotropy effects. At higher temperatures a change of the structure might be expected since the anisotropy weakens with increasing temperatures. Thus the spin system loses its above mentioned ability to constrict the spin structure into a collinear one. This was considered as the reason for the change of the magnetic structure in $TbCu_2$ at $T = 25$ K (the Néel temperature is $T_N = 54$ K). From specific heat and thermal expansion [5] and neutron diffraction experiments [6] it has been found that in most of the RCu_2 intermetallics one or more first- or second-order transitions exist below the corresponding Néel temperatures. It is evident that in addition to the exchange interaction the crystal field is also important for the question of which magnetic structure is stable at a given temperature. It seems that in a first approximation the interplay between anisotropic exchange and crystal field and their temperature dependence are responsible for whether there is a magnetic instability observable in the ordered state or not. Note that there is no magnetic phase transition observable in $GdCu_2$. This supports the assumption that the crystal field is essential for the stability of the magnetic structure. In our recent investigation of $NdCu_2$ we proposed a magnetic phase diagram based on magnetization and specific heat measurements in magnetic fields and on magnetoresistance experiments [7]. In zero magnetic field the magnetic ordering temperature is $T_N = 6.5$ K. In addition we inferred from our experiments a change of the magnetic structure below 4.1 K. In contrast to our findings Svoboda *et al* published a magnetic phase diagram of $NdCu_2$ showing *three* spin reorientations in the ordered state at zero field [8]. The aim of the present investigation was to study whether the two additional magnetic phase transitions at 3.2 K and 5.2 K found by these authors could be confirmed by neutron diffraction and to determine the corresponding magnetic structures. For this a powdered sample was used.

2. Experimental details

A polycrystalline sample of approximately 10 g was obtained by induction melting in a protective Ar atmosphere. After annealing at 700 °C for one week the phase purity was checked by x-ray diffraction and metallographic methods. Within the accuracy of these methods no traces of foreign phases were found.

Powder neutron diffraction experiments were carried out at the multidetector at the SILOE reactor of the Centre d'Etudes Nucléaires de Grenoble (CENG). A graphite monochromator was used ($\lambda = 2.494$ Å) and higher harmonics were removed by a graphite filter.

3. Experimental results

3.1. Nuclear reflections

We first present the results for the chemical structure parameters as deduced from the nuclear reflections. Figure 1 shows the sum of two neutron diffraction patterns of $NdCu_2$ in the paramagnetic state measured at $T = 6.9$ K and 7.7 K. The full curve represents the fit obtained from the Rietveld refinement using the $CeCu_2$ type structure with space group $Imma$ (D_{2h}^{28}, No 74 of the International Tables for Crystallography). The four Nd atoms occupy the equivalent 4e positions (0, 0.25, z); the eight Cu atoms are at the 8h positions (0, y, z) in the elementary cell. The observed and calculated intensities of the nuclear reflections are summarized in table 1. The lattice parameters at 8 K are found to be

$$a = 0.4379(2)\ \text{nm} \qquad b = 0.6993(3)\ \text{nm} \qquad c = 0.7381(3)\ \text{nm}.$$

For the atomic positional parameters we obtain

$$y(\mathrm{Cu}) = 0.0506(4) \qquad z(\mathrm{Cu}) = 0.1670(9) \qquad z(\mathrm{Nd}) = 0.5404(5).$$

These parameters are in good agreement with values obtained by x-ray diffraction on $NdCu_2$ at $T = 10$ K:

$$a = 0.4378 \text{ nm} \qquad b = 0.6997 \text{ nm} \qquad c = 0.7389$$

$$\text{nm}y(\mathrm{Cu}) = 0.0506 \qquad z(\mathrm{Cu}) = 0.1659 \qquad z(\mathrm{Nd}) = 0.5383.$$

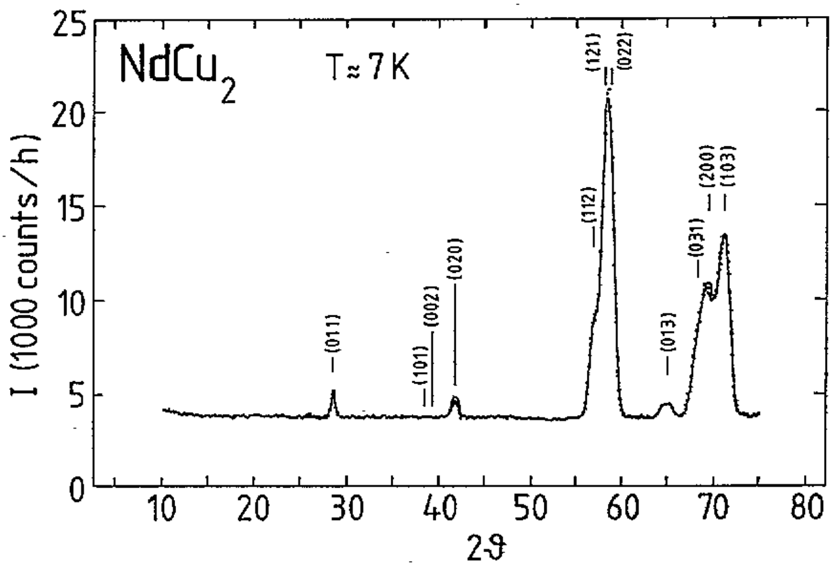

Figure 1. The neutron diffraction pattern of $NdCu_2$ in the paramagnetic state showing the nuclear reflections. The data points are the sum of measurements taken at $T = 6.9$ K and 7.7 K. The full curve represents the result of the Rietveld refinement of the data.

Table 1. The nuclear reflections of $NdCu_2$ in the paramagnetic phase.

(hkl)	2θ	I_{calc}		I_{obs}
(011)	28.44	1816		1844
(101)	38.67	12		—
(002)	39.50	90		—
(020)	41.79	1803		1565
(112)	56.92	12183		12154
(121)	58.24	34894	50385	50603
(022)	58.85	15502		
(013)	65.00	2195		2251
(031)	68.25	12299	62711	62677
(200)	69.44	19347		
(103)	71.09	31076		

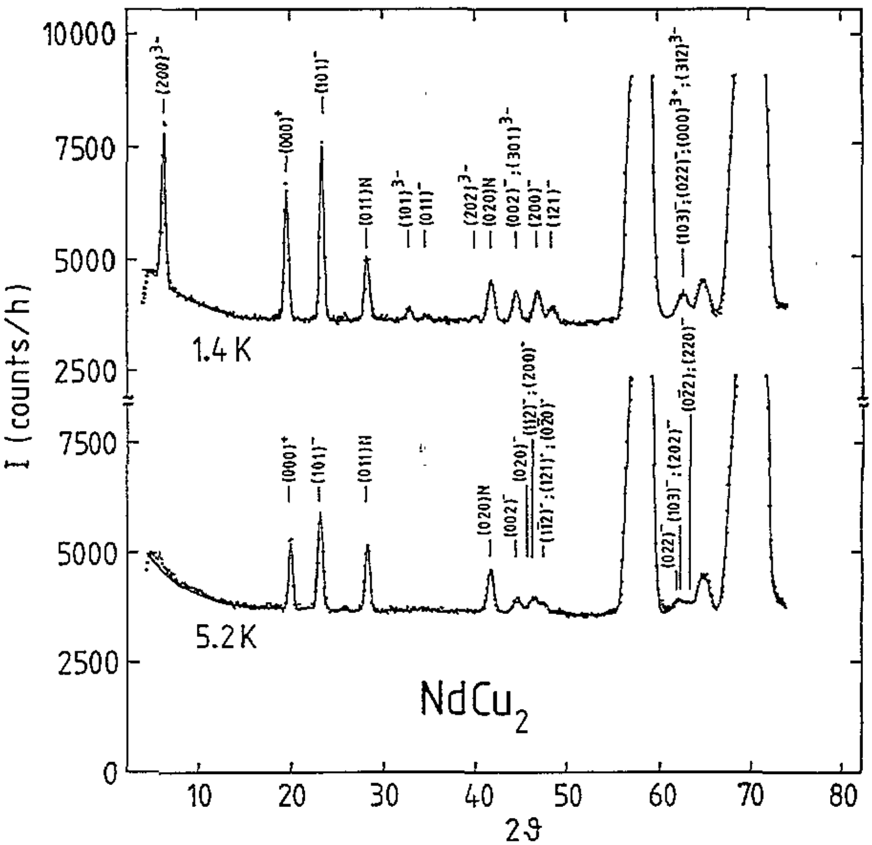

Figure 2. The neutron diffraction pattern of $NdCu_2$ at T = 1.4 K in the commensurate, low-temperature magnetic phase (upper curve) and at 5.2 K in the incommensurate, high-temperature magnetic phase (lower curve). The intensity scale is expanded by a factor of three compared to figure 1. The full curves represent the pattern matching analysis. At 5.2 K the data are described by the wavevector τ^* = (0.612, 0.042, 0), at 1.4 K by, τ = (0.6, 0, 0) and the third harmonic 3τ.

3.2. Magnetic reflections

Below T_N =6.5 K additional, magnetic reflections are observed, indicating that $NdCu_2$ orders antiferromagnetically. In agreement with the phase diagram proposed by Gratz *et al* [7], but in contrast to the phases proposed by Svoboda *et al* [8], we observe in the temperature range from 1.4 K to 6.5 K only two different magnetic phases in zero external field. The lower part of figure 2 shows the diffraction pattern of $NdCu_2$ at T = 5.2 K, which is characteristic of the high-temperature magnetic phase from about 4.3 K up to the ordering temperature of 6.5 K. Compared to figure 1 the intensity scale has been enlarged by a factor of three to make the various magnetic reflections clearly visible. No significant change in the peak positions and intensities of the nuclear reflections is observed for all patterns between 1.4 K and 7.7 K. The magnetic reflections in the high-temperature region can be indexed using a single wavevector, τ^*, indicating a sinusoidal modulation. The full curve shows the pattern matching analysis using the wavevector τ^* = (0.612, 0.042, 0). The determination of this wavevector will be discussed in more detail later in this section. Accordingly, in the high-temperature phase the magnetic structure is incommensurate with the lattice. The

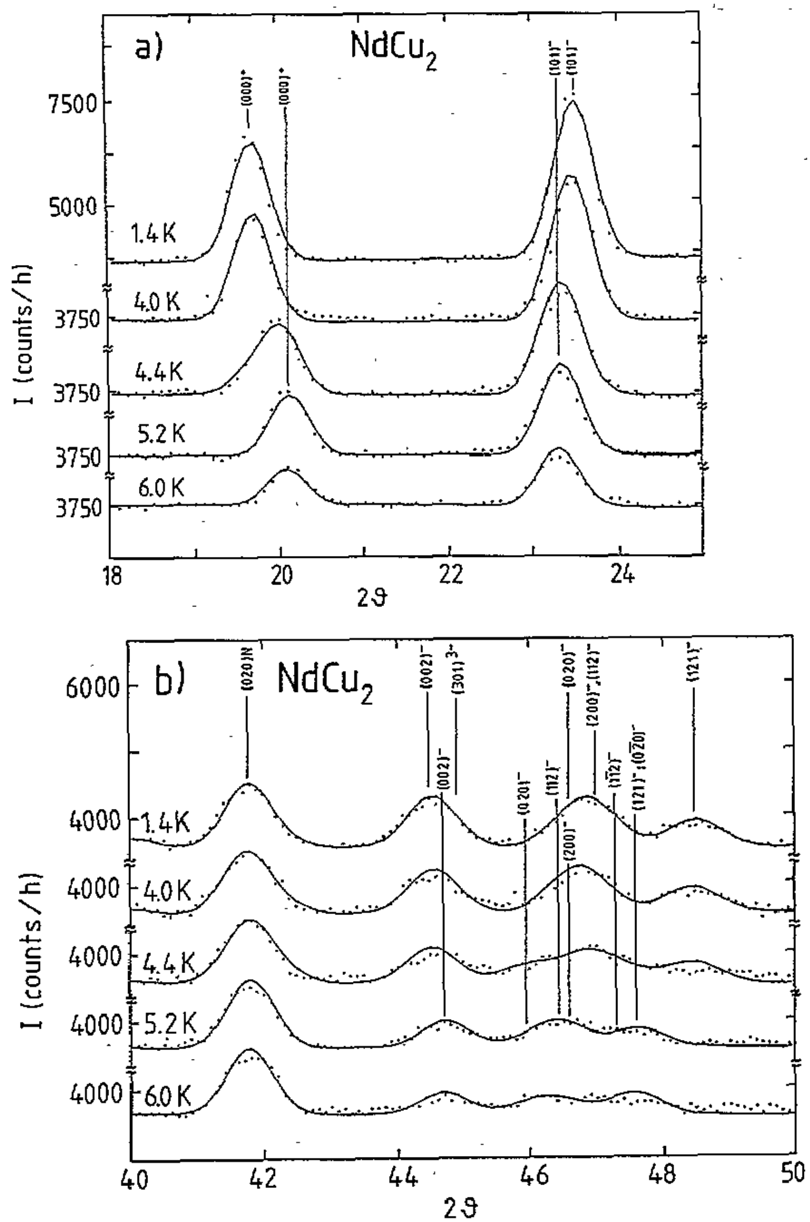

Figure 3. The temperature dependence of the reflections in the 2θ range (a) from 18° to 25° and (b) from 40° to 50°. The full curves represent the pattern matching analysis of the data: at 1.4 K and 4.0 K the wavevector $\tau = (0.6, 0, 0)$ and the third harmonic 3τ are used; the data at 5.2 K and 6.0 K are described by the wavevector $\tau^* = (0.612, 0.042, 0)$; the full curve for T = 4.4 K represents a superposition of the wavevectors in the low- and high-temperature phases.

peak positions of the magnetic reflections are summarized in table 2. The upper part of figure 2 shows the diffraction pattern of NdCu$_2$ at T = 1.4 K, which is typical of the low-temperature phase up to at least 4.0 K. Compared with the high-temperature phase, two different features are evident. At first a clear shift in the positions of the original reflections is observed: e.g. the position of the $(0\,0\,0)^+$ varies from $2\theta = 20.09°$ in the high-temperature phase to $2\theta = 19.68°$ in the low-temperature phase (see figure 3). From the pattern matching analysis it follows that the wavevector, τ, in the low-temperature phase is given by $\tau = (0.6, 0, 0)$, so the magnetic structure becomes commensurate with the lattice. Apart from the reflections determined by the fundamental modulation, τ, additional reflections appear, which can be described by the third harmonic, 3τ. Accordingly, in the commensurate phase a progressive squaring up of the sinusoidal modulation is observed in the range from 4.0 K down to 1.4 K (see also figure 4). The strong peak at $2\theta \simeq 6.5°$ represents the $(2\ 0\ 0)^{3-}$. On the other hand, the $(0\ 0\ 0)^{3+}$, which appears at $2\theta = 61.68°$, is nearly hidden by various reflections of the fundamental modulation in this region. However, preliminary single-crystal measurements show unambiguously that the $(0\ 0\ 0)^{3+}$ is also present in the low-temperature phase. The peak positions of the various magnetic reflections in the low-temperature phase are given in table 3.

Table 2. The magnetic and nuclear reflections of $NdCu_2$ in the high-temperature phase at T = 5.2 K.

(hkl)	2θ	I_{calc}		I_{obs}
$(000)^+$	20.09	1790		1684
$(101)^-$	23.31	2506		2632
(011)N	28.44	1816		1956
$(011)^-$	34.54	50		137
$(0\bar{1}1)^-$	35.60	45		92
(101)N	38.67	12		6
(002)N	39.50	90		85
(020)N	41.79	1803		1729
$(002)^-$	44.70	579		694
$(020)^-$	45.95	71		157
$(112)^-$	46.46	130	478	666
$(200)^-$	46.58	348		
$(1\bar{1}2)^-$	47.30	122		
$(121)^-$	47.58	157	341	518
$(0\bar{2}0)^-$	47.63	62		
$(1\bar{2}1)^-$	49.22	138		0
$(211)^-$	55.11	27		
$(2\bar{1}1)^-$	55.85	26		
(112)N	56.92	12183		12824
(121)N	58.24	34894		33877
$(\bar{1}01)^-$	58.58	428	15930	16543
(022)N	58.85	15502		
$(022)^-$	62.16	171		
$(103)^-$	62.51	217	699	901
$(202)^-$	62.68	311		
$(0\bar{2}2)^-$	63.54	158	268	554
$(220)^-$	63.67	110		
(013)N	65.00	2295	2398	2547
$(2\bar{2}0)^-$	65.03	1-3		
(031)N	68.25	12299	12446	13276
$(013)^-$	68.47	147		
$(0\bar{1}3)^-$	69.13	142	19489	17897
(200)N	69.44	19347		
(103)N	71.09	31076		31681

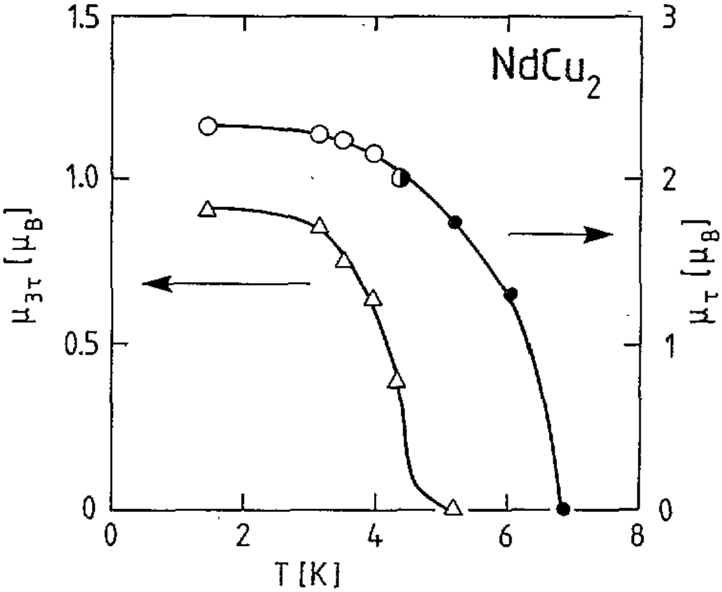

Figure 4. The temperature dependence of the amplitudes of the three oscillating components in the two magnetic phases of $NdCu_2$: ○ for $\tau = (0.6, 0, 0)$ and △ for 3τ in the low-temperature phase; ● for $\tau^* = (0.612, 0.042, 0)$ in the high-temperature phase. The half open circle represents the mixed phase region at $T = 4.4$ K; note the presence of the third harmonic 3τ at this temperature.

The temperature dependence of two groups of magnetic reflections is shown in figure 3. From the clearly visible shift of the $(0\,0\,0)^+$ and the $(1\,0\,1)^-$ reflections from their 2θ values in the low-temperature phase, it follows that the wavevector in the high-temperature phase must deviate from the commensurate value of $\tau = (0.6, 0, 0)$. However, by varying only the a-component of the wavevector we were unable to obtain a correct description of the group of reflections in the 2θ range between 40° and 50°. With the wavevector $\tau^* = (0.612, 0.042, 0)$, a rather satisfactory fit of the high-temperature diffraction pattern is obtained, as is seen in figure 3(b). The presence of a small b-component in the high-temperature phase is confirmed by single-crystal data. On the other hand, neither in the low-temperature phase, presented by the data at $T = 1.4$ K and $T = 4.0$ K, nor in the high-temperature phase, as is seen for $T = 5.2$ K and $T = 6.0$ K, is any shift of the magnetic satellites observed. Therefore, we believe that only two magnetic structures of $NdCu_2$ exist in zero external field with temperature independent wavevectors, τ and τ^*, in the low- and high-temperature phases, respectively. The diffraction pattern at $T = 4.4$ K seems to show an intermediate phase. However, the data can also be fitted assuming a mixture of the two phases. This is demonstrated by the curves drawn for 4.4 K in figure 3, which represent a superposition of the two wavevectors of the low- and high-temperature phases. The fact that the third harmonic is retained up to 4.4 K also seems to support this idea (see figure 4).

3.3. Magnetic structure

In order to determine the magnetic structure in the two magnetic phases, we need to include the observed intensities of the various reflections. The data at 5.2 K in the high-temperature phase are summarized in table 2, those at 1.4 K in the low-temperature phase in table 3. In

Table 3. The magnetic and nuclear reflections of $NdCu_2$ in the low-temperature phase at $T = 1.4$ K.

(hkl)	2θ	I_{calc}		I_{obs}
$(200)^{3-}$	6.53	4510		4065
$(000)^{+}$	19.68	3324		3286
$(101)^{-}$	23.51	4384		4520
(011)N	28.44	1816		1878
$(211)^{3-}$	29.22	28		168
$(101)^{3-}$	32.95	340		425
$(011)^{-}$	34.83	170		166
(101)N	38.67	12		17
(002)N	39.50	90		19
$(202)^{3-}$	40.08	191		212
(020)N	41.79	1803		1591
$(220)^{3-}$	42.35	5		142
$(002)^{-}$	44.50	1038		1058
$(301)^{3-}$	44.82	188		333
$(020)^{-}$	46.60	231		472
$(200)^{-}$	46.99	608	1056	1090
$(112)^{-}$	47.00	447		
$(121)^{-}$	48.51	529		782
$(112)^{3-}$	52.83	57		0
$(121)^{3-}$	54.22	102		17
$(211)^{-}$	55.85	92		—
(112)N	56.92	12183		11620
$(\bar{1}01)^{-}$	58.15	771	51255	50997
(121)N	58.24	34894		
(022)N	58.85	15502		
$(222)^{3-}$	59.29	88		
$(000)^{3+}$	61.68	56	101	0
$(312)^{3-}$	61.68	45		
$(103)^{-}$	62.60	386	1628	1504
$(022)^{-}$	62.69	586		
$(321)^{3-}$	62.95	108		
$(202)^{-}$	63.02	548		
$(220)^{-}$	64.68	378	2756	2267
(013)N	65.00	2295		
$(213)^{3-}$	65.41	83		
$(103)^{3-}$	67.52	51		0
(031)N	68.25	12299	32161	30514
$(013)^{-}$	68.65	515		
(200)N	69.44	19347		
(103)N	71.09	31076		30828

both phases the $(2h\ 0\ 0)\pm$ reflections are present; this implies that the Nd moments within each b–c plane must be aligned ferromagnetically. In both phases the intensities can be reproduced by assuming a sinusoidal oscillation of the Nd moments, which are oriented along the b-direction. This is the direction favoured by the crystal field anisotropy at low temperatures [7]. Accordingly, the structure factor is given by

$$|F_M|^2 = (\tfrac{1}{4})(e^2\gamma/2mc^2)^2\mu^2 \sin^2\alpha. \qquad (1)$$

Here the constant $(e^2\gamma/2mc^2) = 0.2695 \times 10^{-12}$ cm, α is the angle between the scattering vector $(hkl)^{\pm}$ and the direction of the magnetic moment and μ is the amplitude of the oscillation in μ_B. In the high-temperature phase the wavevector is nearly along the a-direction; accordingly, we obtain a nearly transversely oscillating component. Table 2 contains the observed and calculated intensities at 5.2 K in the high-temperature phase. The calculated intensities correspond to a sinusoidal oscillation of amplitude 1.74 (10)μ_B for the Nd moments along the b-direction. The magnetic form factor, f, is taken as isotropic and is approximated by $f^2 = \exp[-(Q(\text{Å}^{-1})/6.6)^2]$.

In the low-temperature phase the wavevector is exactly along the a-direction, so a completely transversely oscillating component is obtained. The observed and calculated intensities of the various magnetic reflections at 1.4 K are given in table 3. The calculated intensities correspond to a modulation amplitude of 2.32 (10)μ_B for the fundamental oscillation τ and 0.90 (10)μ_B for the third harmonic 3τ at 1.4 K. In figure 4 we have plotted these two amplitudes as a function of temperature, together with the amplitude of the sinusoidal oscillation in the high-temperature phase. Within the accuracy of the measurements no clear discontinuity in the amplitudes of the fundamental oscillations seems to occur at the phase transition around 4.4 K. The contribution of the higher harmonic has not yet completely disappeared at 4.4 K, which supports our proposal about the coexistence of the two phases at this temperature.

Now we want to conclude our discussion on the magnetic structure at the lowest temperature of 1.4 K. The Nd moments are arranged in ferromagnetic b–c sheets and the distance between the adjacent sheets is $a/2$, so the magnitude of the moment in each sheet is given by $\mu = \mu_\tau \sin(2\pi\tau R_i/a+\phi_1)+\mu_{3\tau}\sin(6\mu\tau R_i/a+\phi_3)$, where $R_i = 0, a/2, a, \ldots, 5a$. Accordingly, the modulation is repeated after 10 sheets. From the diffraction data at 1.4 K the amplitudes are found to be $\mu_\tau = 2.3\mu_B$ and $\mu_{3\tau} = 0.9\mu_B$. However, no information about the phase angles ϕ_1 and ϕ_3 can be obtained from a neutron diffraction experiment. Accordingly, the magnetic structure determined by these two phases cannot be deduced unambiguously from a neutron diffraction experiment alone. Without any information from other experiments, the assignment of the phases can only be based on arguments as to which model is most reasonable. This problem has been extensively discussed in the past and an instructive example in order to solve the commensurate magnetic structure of NpP can be found in [9]. In our case of NdCu$_2$ no conditions imposed from other experiments have to be considered. For an arbitrary choice of ϕ_1 and ϕ_3 the values in five successive planes would be all different. On the other hand it is expected that the appearance of the third harmonic arises from the squaring up of the magnetic structure. Some squaring up can be obtained already by considering these two modulations only. For this they should be as out of phase as possible. A rather symmetric moment configuration along the a-direction is obtained for $\phi_1 = 0.3\pi$ and $\phi_3 = 0.9\pi$. It is readily calculated that in this case only two values of the magnetic moment, i.e. $1.4\mu_B$ and $2.15\mu_B$ are obtained and that the average moment in the fivefold-enlarged cell is about $1.72\mu_B$. On the other hand, the easiest way of arguing is the following. In the case of complete squaring up all higher harmonics should be present with amplitudes $\mu_{3\tau}/\mu_\tau = \frac{1}{3}$, $\mu_{5\tau}/\mu_\tau = \frac{1}{5}$, $\mu_{7\tau}/\mu_\tau = \frac{1}{7}, \ldots$, while their phases would be given by $\phi_1 = \pi/2$, $\phi_3 = -\pi/2$, $\phi_5 = \phi/2$, $\phi_7 = -\pi/2$ and so forth. Accordingly, the ratio of the experimental values $\mu_\tau = 2.3\mu_B$ and $\mu_{3\tau} = 0.9\mu_B$ at 1.4 K agrees with that expected for complete squaring up. This means that reflections arising from the fifth harmonic should also appear and we will now discuss whether these reflections might be seen. The $(3\ 0\ 1)^{5-}$ would appear at $2\theta = 19.45°$; from the theoretical value of $\mu_{5\tau}/\mu_\tau = \frac{1}{5}$ its intensity is expected to be 255. Its presence would be completely hidden by the strong $(0\ 0\ 0)^+$ peak at $2\theta = 19.68°$. Apart from this reflection, only the intensity of the combined $(2\ 0\ 0)^{5-}$ and $(4\ 0\ 0)^{5-}$ reflection would be sufficiently strong (nearly 100) to be visible. However, due to its location at $2\theta = 33.09°$, it coincides with the $(1\ 0\ 1)^{3-}$, which prevents a separation of the two contributions. Thus from our powder work it cannot be concluded whether the fifth harmonic is present or not. On the other hand, its presence is confirmed from our single-crystal work. Therefore we believe that the assumption of complete squaring up is justified. In figure 5(a) we have drawn schematically the arrangement of the magnetic moments for the squared up structure at 1.4 K. Each arrow represents a ferromagnetic b–c plane and the distance between adjacent planes is $a/2$. The squared up structure represents the superposition of the fundamental oscillation with wavevector τ = (0.6, 0 0) and the higher harmonics, as described before. For comparison we have drawn in figure 5(b) the magnitudes of the magnetic moments in the case where only the fundamental is present. The dashed lines indicate zero values of the sinusoidal modulation. Using the Fourier series described above, the amplitude of the square wave is calculated to be $(\pi/4)2.3\mu_B \simeq 1.8\mu_B$.

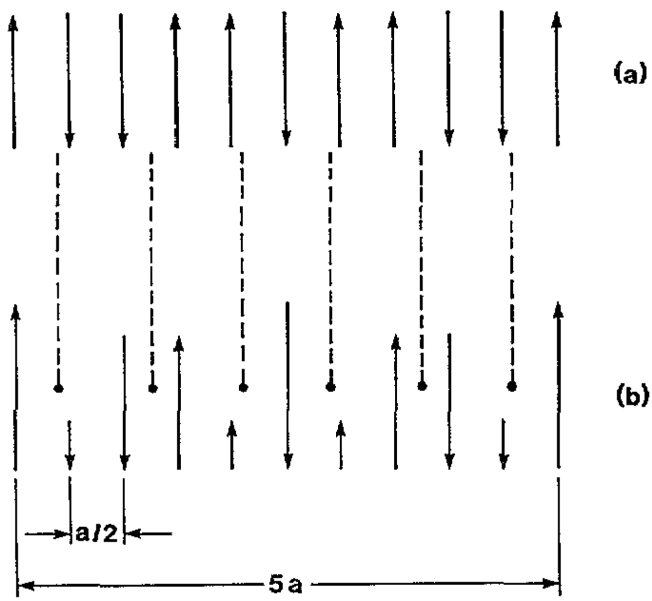

Figure 5. (a) A schematic diagram drawing of the squared up magnetic structure of $NdCu_2$ at 1.4 K, due to the additional appearance of the higher harmonics of the wavevector τ = (0.6, 0, 0). For comparison the structure arising from the fundamental modulation alone has also been drawn in (b); the dashed lines represent the zero values of this sinusoidal modulation. Each arrow represents the magnitude of the moment in a ferromagnetic b–c plane, the distance between adjacent planes is $a/2$, and the modulation is repeated after 10 planes. For the squared up structure the value of each moment is about $1.8\mu_B$, while for the sinusoidal modulation the *maximum value of* $2.3\mu_B$ *is obtained.*

As is seen in table 3, of the three reflections $(2\ 0\ 0)^-$, $(0\ 2\ 0)^-$, and $(0\ 0\ 2)^-$, the first is the strongest, while the $(0\ 2\ 0)^-$ is the weakest reflection in agreement with $\tau \parallel a$ and $\mu \parallel b$ (see (1)). From this it is clear that the unambiguous determination of the transversely oscillating component is related to the low crystallographic symmetry with $a \neq b \neq c$ in $NdCu_2$, which leads to different d-spacings for the three magnetic reflections involved. On the other hand, if the system were cubic the $(0\ 2\ 0)^-$ and $(0\ 0\ 2)^-$ reflections would coincide for $\tau \parallel a$ in a powder diffraction experiment and we would not be able to distinguish between a transversely oscillating component and a helical structure.

Finally we would like to emphasize that at first glance the strong reflection at $2\theta \simeq 6.5°$ in the low-temperature phase might be also ascribed to the $(0\ 0\ 0)^+$ of the wavevector (0.2, 0, 0). Accordingly, the wavevector (0.6, 0, 0) would then be the third harmonic. In that case the amplitude of the fundamental oscillation would be weaker than that of the third harmonic, which seems to be physically unrealistic. Such a behaviour was recently reported for the low-temperature phase of $TmCu_2$ [10], though the structure seems to be similar to that of $NdCu_2$. By choosing the wavevector (0.6, 0, 0) as the fundamental oscillation, as done in our present work, the correct description for the two amplitudes is obtained; additionally, the fundamental wavevector changes only slightly from incommensurate into commensurate at the second phase transition.

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