THE MODULATED STRUCTURE OF NEODYMIUM CRYSTAL
A. Jaroszewicz, P. Kociski, G. Tecza, J. Kociski

To cite this version:

HAL Id: jpa-00228298
https://hal.archives-ouvertes.fr/jpa-00228298
Submitted on 1 Jan 1988

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
THE MODULATED STRUCTURE OF NEODYMIUM CRYSTAL

A. Jaroszewicz (1), P. Kociński (1), G. Tecza (1) and J. Kociriski (2)

(1) Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 36/42, Warszawa, Poland
(2) Warsaw Technical University, Institute of Physics, Koszykowa 75, 00-662 Warszawa, Poland

Abstract. — Applying Landau’s theory we have determined the spin structure of neodymium crystal below \( T_c = 19.3 \) K for the star of the vector \( q_1 = \mu_1 b_1 + \mu_2 b_2 \), \( -0.5 < \mu_1, \mu_2 < 0.5 \), \( \mu_1, \mu_2 \neq 0 \). The corresponding cross-section for magnetic scattering of polarized neutrons yields the satellites \( h \pm q_1, 0, 0 \). Two pairs of satellites around the point \( (0, 1, 0) \) have lower intensities than the remaining ones.

The crystal structure of Nd is dhcp with a four layer stacking sequence along the \( a_3 \)-axis of type ABAC. The phase transition at the temperature \( T = 19.3 \) K is connected with the vector \( q_1 = \mu_1 b_1 + \mu_2 b_2 \), \( -0.5 < \mu_1, \mu_2 < 0.5 \), \( \mu_1, \mu_2 \neq 0 \), \( b_1 \) and \( b_2 \) are the reciprocal lattice vectors [1]. This transition is calculated as if it occurred from the paramagnetic phase and not from the intermediate magnetically ordered phase which appears below \( T = 19.9 \) K [2].

The star of \( q_1 \) consists of twelve vectors: \( q_1, \ldots, q_{12} \), which are obtained from \( q_1 \) under the action of the rotations \( R_i \), \( i = 1, \ldots, 12 \), numbered according to Kovalev [3]. The isotropy co-group of \( q_1 \) is \( m \) and it has two real projective representations \( \hat{\tau}_1 \) and \( \hat{\tau}_2 \) which are Landau active. The group generator matrices for the two full representations \( \Gamma_1, \Gamma_2 \) induced on the basis of Kovalev’s formula [3] from \( \hat{\tau}_1 \) and \( \hat{\tau}_2 \), respectively, are:

\[
\Gamma(R_2 | \tau_R) = \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix}
\]
\[
\Gamma(R_7 | 0) = \begin{bmatrix} 0 & B \\ B & 0 \end{bmatrix}
\]
\[
\Gamma(R_{12} | 0) = \pm \begin{bmatrix} C & 0 \\ 0 & C \end{bmatrix}
\]

where:

\[
A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}
\]

\[
B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}
\]

\[
C = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}
\]

and where the "-" sign corresponds to \( \Gamma_2 \) representation.

The thermodynamic potential accurate to the sixth-degree invariants constructed from the expansion coefficients \( c_j \) of the order parameter \( S(x) = \sum c_j \Psi_j(x) \) (\( \Psi_j \) are the basis functions) consists of eleven terms. Since under the internal translations the expansion coefficients transform like \( t_n c_j = c_j \times \exp(-i q_j \cdot t_n) \), where \( q_j \) are the star vectors, those invariants can only be constructed from the expressions: \( c_1 c_4, c_2 c_5, c_3 c_6 \), \( c_7 c_10, c_8 c_11, c_9 c_12, c_1 c_8 c_5, c_2 c_4 c_6, c_7 c_9 c_11, c_6 c_10 c_12 \). To the minima of the thermodynamic potential density correspond sets of solutions consisting of one, two, three, four, five or six pairs of non-zero \( c_j \) with the coefficients \( c_j, c_{j+3}, j = 1, 2, 3, 7, 8, 9 \), appearing together.

In order to determine the spin structure we need the basis functions. Applying the projection operator to the trial function:

\[
f(r) = \sum_{n=1}^{N} \begin{bmatrix} d_{n1} \\ d_{n2} \\ d_{n3} \end{bmatrix} e^{i(q_1 \cdot r + p_n b_3 r + \Delta_n a_3 \cdot b_3)}
\]

where \( N = \) positive integer, \( q_1 \) is the first vector of the star, \( d_{nj}, j = 1, 2, 3 \), are complex components referred to the oblique axes \( x_1, x_2, x_3 \) parallel to respective basis vectors of Bravais lattice, \( b_3 \) is the reciprocal lattice vector, \( p_n \) are integers, \( \Delta_n \) are numerical parameters, we obtain six pairs of complex basis functions, each pair connected with \( \pm q_1, j = 1, \ldots, 6 \). Calculations indicate that the representation \( \Gamma_1 \) and \( \Gamma_2 \) lead to spin structures of the same type. For the representation \( \Gamma_2 \)
the spin structure at the lattice site \( \mathbf{r} \) is:

\[
S(\mathbf{r}) = \sum_{n=1}^{N} \sum_{j=1}^{6} \left\{ \mu_{j,n} \xi_j \sin[p_n b_3 \cdot \mathbf{r} + 2\Pi \Delta_n - p_n \Pi/2] \times \cos[\xi_j p_n b_3 \cdot \mathbf{r} + 2\Pi \Delta_n - p_n \Pi/2] + \xi_j \mu_{j,n} \sin[p_n b_3 \cdot \mathbf{r} + 2\Pi \Delta_n - p_n \Pi/2] \times \sin[\xi_j p_n b_3 \cdot \mathbf{r} + 2\Pi \Delta_n - p_n \Pi/2] \right\}
\]

(4)

where \( \xi_1 = \xi_3 = \xi_5 = -\xi_2 = -\xi_4 = -\xi_6 = 1 \). To obtain "1 - q", "2 - q", ..., "6 - q" structure we retain in the sum over \( j \) one, two, ..., six terms, respectively. The vectors \( \mu_{j,n} \) are:

\[
\begin{align*}
\mu_{1,n} &= 2\eta_i \begin{bmatrix} d_{n1} \\ d_{n2} \end{bmatrix} & \mu_{r,n} &= 2\eta_i \begin{bmatrix} -d_{n1} \\ 0 \end{bmatrix} \\
\mu_{2,n} &= 2\eta_i \begin{bmatrix} -d_{n1} + d_{n2} \\ 0 \end{bmatrix} & \mu_{s,n} &= 2\eta_i \begin{bmatrix} -d_{n2} \\ -d_{n1} \end{bmatrix} \\
\mu_{3,n} &= 2\eta_i \begin{bmatrix} d_{n2} - d_{n1} \\ 0 \end{bmatrix} & \mu_{g,n} &= 2\eta_i \begin{bmatrix} -d_{n2} + d_{n1} \\ 0 \end{bmatrix} \\
\mu_{5,n} &= 2\eta_i d_{n3} \begin{bmatrix} 0 \\ 0 \end{bmatrix} & \mu_{z,n} &= 2\eta_i d_{n3} \begin{bmatrix} 0 \\ 1 \end{bmatrix}
\end{align*}
\]

(5)

where now \( d_{n1}, d_{n2}, d_{n3} \) are imaginary.

According to experiment [1], the spin vectors deviate from the q directions which also follows from equation (4). The measured effects [1, 4, 5] are obtained for the spin structure equation (4) with the following values of the parameters:

\[
N = 3, \quad p_1 = p_2 = p_3 = 1, \quad \Delta_1 = 0, \quad \Delta_3 = -\Delta_2 = -\frac{1}{4}, \quad d_{32} = d_{31} = d_{12} = d_{23} = 0.
\]

(6)

From equations (3), (4), (5) we obtained the following cross-section for the elastic magnetic scattering of polarized neutrons:

\[
\frac{d\sigma}{d\Omega} \sim \sum_{\tau} \sum_{j=1}^{6} \left[ \delta(\tau - \kappa + q_j) L_+^{(j)}(\tau) + \delta(\tau - \kappa - q_j) L_-^{(j)}(\tau) \right]
\]

(7)

where:

\[
L_\pm^{(j)}(\tau) = \left[ \mu^2_{H,j} - (\mathbf{e} \cdot \mathbf{\mu}_{C,j})^2 \right] (1 - \cos \pi l)
\]

\[
+ \left[ \mu^2_{H,j} - (\mathbf{e} \cdot \mathbf{\mu}_{H,j})^2 \right] \left\{ 1 - \cos \pi \left[ l - \frac{2}{3} (h - k) \right] \right\}
\]

\[
+ \left[ \mu^2_{C,j} - (\mathbf{e} \cdot \mathbf{\mu}_{C,j})^2 \right] (1 - \cos \pi l)
\]

\[
\mp \left[ \mu_{H,j} \mu_{C,j} - (\mathbf{e} \cdot \mathbf{\mu}_{H,j}) (\mathbf{e} \cdot \mathbf{\mu}_{C,j}) \right] 4 \sin(\pi l/2)
\]

\[
\times \cos(\pi (h + k) \cos \pi (h - k) / 3
\]

\[
+ \mathbf{P} \left[ \mu_{C,j} \times \mu_{H,j} - (\mathbf{e} \cdot \mathbf{\mu}_{C,j}) \mathbf{\mu}_{C,j} \times \mathbf{e} \right]
\]

\[
\times 4 \sin(\pi l/2 \cos \pi (h + k) \cos \pi (h - k) / 3)
\]

\[
\mp \mathbf{P} \left[ \mu_{C,j} \times \mu_{C,j} - (\mathbf{e} \cdot \mathbf{\mu}_{C,j}) \mathbf{\mu}_{C,j} \times \mathbf{e} \right] (1 - \cos \pi l)
\]

(8)

where the vectors \( \mu_{H,j}, \mu_{C,j}, j = 1, \ldots, 6 \), and \( \mu_z \) from equation (5) now are referred to the Cartesian system of coordinates \( x, y, z \), with the \( z \)-axis parallel to the \( x_3 \) axis; \( \tau = h b_1 + k b_2 + l b_3 \) denotes an integral reciprocal lattice vector, \( \kappa \) is the scattering vector, \( \mathbf{e} \) is equal to \( \kappa / \kappa \) and \( \mathbf{P} \) is the polarization vector of the incident neutron beam. The cross-sections for "single-q", "double-q", "triple-q", "quadruple-q" or "quintuple-q" spin structure are obtained from equations (7), (8) when we retain one, two, three, four or five terms in the sum over \( j \) in equation (7), respectively.

The cross-section equations (7), (8) has the following features: (1) the \( (x, y) \)-components of spin on the "cubic sites" contribute to the cross-section only for \( l \) odd; (2) the \( (x, y) \)-components of spin do not contribute to the cross-section for \( l \) even and \( h - k = 3n \) with \( n \) integer; (3) for \( l \) odd replaced by \( l + 2n \) with \( n \) odd the signs in front of the double sign terms in equation (7) change from \( \mp \) to \( \pm \) (4) both \( (\mp) \)-terms vanish for \( l \) even; (5) there are no satellites around the points \( (0, 0, 0) \) and \( (1, 1, 0) \); (6) owing to the factor \( \left[ \mu^2_{H,j} - \mathbf{e} \cdot \mathbf{\mu}_{H,j} \right] \) in the second term of equation (8) the twelve satellites around the point \( (h, 0, 0) \) are absent; (7) the polarization-dependent terms influence the reflected intensity only for \( l \) odd; (8) the \( (h \pm g, 0, 0) \) satellites are permitted; (9) for the parameter values given in equation (6) and for \( d_{12} = d_{21} \) the satellites around the point \( (0, 1, 0) \) connected with \( q_3, q_6, q_7, q_{10} \) have lower intensity than the remaining eight ones.

The properties of the cross-section equations (7), (8) listed in the points (1) to (9) agree with experiment [1, 5].