HELICAL SPIN STRUCTURES IN c-AXIS Dy/Y SUPERLATTICE*

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On the basis of Landau's theory of symmetry changes at continuous phase transitions, we have derived the formulae for two incommensurate helical spin structures which are symmetry allowed in Dy/Y superlattice, when the helical axis is parallel to the c-axis of the hexagonal lattice. These structures have different extinction coefficients in their cross-sections for magnetic scattering of neutrons and therefore can be distinguished by experiment. Magnetic satellite peaks around the reciprocal lattice points $\boldsymbol{K}+\mathbf{0}$ are allowed for only one of these spin structures, namely that inferred from earlier experiments.

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1. Introduction

The existence of a helical spin structure in single crystal Dy/Y superlattices, with the growth plane of the bilayers perpendicular to the sixfold symmetry axis of bulk Dy or Y crystals, was inferred from the experiment of Erwin et al. [1]. From the type of the measured magnetic peaks, a phase coherence of the spin helix in the successive Dy layers across the non-magnetic Y layers was deduced. An analogous situation was stated by Giebułtowicz et al. [2] for the magnetic semiconductor MnSe/ZnTe superlattice, when the respective helical axis is parallel to the z-direction. In the latter case the coherence of the spin structure of the MnSe layers across the non-magnetic ZnTe layers was explained by considering the resultant symmetry of the superlattice [3]. The method of calculation introduced in Ref. [3] can be carried out for the Dy/Y superlattice. On this basis a theoretical deduction of the spin structure from Ref. [1] and of the respective magnetic neutron scattering cross-section will be given. They have not been derived in other papers.

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2. Method of calculation

Single crystals of Dy or Y have a hexagonal closed packed structure. Due to the lattice constant mismatch in the basal plane of the hexagonal lattice which is the growth plane of the superlattice, the Dy layers are compressed to fit with the lattice-site spacing of the Y layers [1]. The superlattice represents a single crystal, consisting of a certain number of Dy/Y bilayers, each of a thickness L. Each bilayer consists of a fixed number of Dy and Y atomic planes (Fig. 1). We

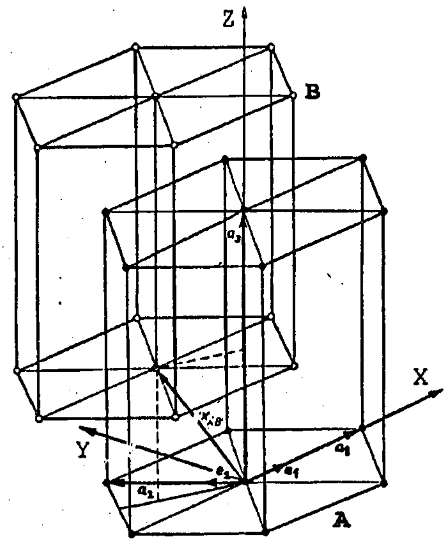

Fig. 1. The positions of Dy atoms in the two simple hexagonal lattices A and B, and the Cartesian system of axes x, y, z. The group centre is at the origin of coordinates.

shall assume that the projections on the growth plane of the respective Dy and Y atoms coincide. The superlattice then is characterized by the lattice constants $a_1(\mathrm{Dy}) = a_1(\mathrm{Y})$, $a_2(\mathrm{Dy}) = a_2(\mathrm{Y})$, with $|a_1| = |a_2|$ and $a_3(\mathrm{Dy}) \neq a_3(\mathrm{Y})$ in the direction perpendicular to the layer plane. The unit cell of the superlattice then is determined by the following vectors:

$$a_1 = (a, 0, 0), \quad a_2 = (0, a, 0), \quad a_L = (0, 0, L), \tag{2.1}$$

where L is the layer thickness. We assume an odd number of Dy atomic planes in a Dy/Y bilayer which corresponds to the experiment in Ref. [1]. The Cartesian coordinate axes and the group centre are represented in Fig. 1. The bilayer structure of the superlattice implies a decrease in the resultant symmetry in comparison with the bulk crystal symmetry of Dy or Y. The resultant space group symmetry of the Dy/Y superlattice is $P3m(C_{3v}^1)$.

3. Spin structure

We consider continuous magnetic phase transitions of the superlattice from the paramagnetic phase of symmetry $P3m1'$, where $1'$ denotes the time-reversal group, induced by the irreducible representations (irreps) at the point determined by the wave vector

$$\boldsymbol{k}_1 = \nu \boldsymbol{b}_L, \quad -0.5 < \nu < 0.5, \quad \nu \neq 0. \tag{3.1}$$

The wave vector is chosen on the basis of the experiment from Ref. [1], where the helical axis is parallel to the z-direction. The star of $\boldsymbol{k}_1$ has one arm and therefore the point group $G_{\boldsymbol{k}0}$ connected with the little group of $\boldsymbol{k}_1$ contains the rotational elements of the high-temperature crystallographic symmetry group $P3m$. In Kovalev's Tables [4] we find three projective irreps of the point group $G_{\boldsymbol{k}0}$ given in Table. The representation τ_3 does not fulfil Kovalev's condition [6, 7] and it

TABLE

The projective irreps τ_1, τ_2, τ_3 from Ref. [4] with $u = \exp(2\pi i/3)$. The rotational elements are numbered as in Ref. [4] and the respective symbols in the brackets are from Ref. [5].

	$R_3(C_3^+)$	$R_5(C_3^-)$	$R_{19}(\sigma_{v2})$	$R_{21}(\sigma_{v1})$	$R_{23}(\sigma_{v3})$
τ_1	1	1	1	1	1
τ_2	1	1	−1	−1	−1
τ_3	$\begin{pmatrix} u & 0 \\ 0 & u^2 \end{pmatrix}$	$\begin{pmatrix} u^2 & 0 \\ 0 & u \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & u \\ u^2 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & u^2 \\ u & 0 \end{pmatrix}$

cannot be active. The irreps τ_1 and τ_2, which fulfil Kovalev's condition and weak Lifshitz condition (since the vector $\boldsymbol{k}_1$ has one degree of freedom and there exists only one Lifshitz invariant), are active and it can be shown that they both induce transitions to the helical spin structure of the type inferred from the experiment.

We will perform the calculations for the irrep τ_2. The respective calculation for the irrep τ_1 is exactly analogous. The full irrep Γ_2 of the space group $P3m$ is the same as that of the little group $G_{\boldsymbol{k}}$. The integral translation elements $\boldsymbol{t}_n$ are represented by the exponential terms: $\exp(-i\boldsymbol{k}_1 \cdot \boldsymbol{t}_n)$, $\boldsymbol{t}_n = n_1\boldsymbol{a}_1 + n_2\boldsymbol{a}_2 + n_3\boldsymbol{a}_L$, n_j — integer, $j = 1, 2, 3$. The spin structure $\boldsymbol{S}(\boldsymbol{r})$ is determined by the basis function $\Psi(\boldsymbol{r})$ of the irrep Γ_2 in the following form:

$$\boldsymbol{S}(\boldsymbol{r}) = c\Psi(\boldsymbol{r}), \tag{3.2}$$

where the coefficient c is determined from the minimum conditions of the respective thermodynamic potential.

The thermodynamic potential density can be written in the form

$$\Phi = \Phi^{(0)} + A|c|^2 + B|c|^4, \tag{3.3}$$

where $A \propto (T - T_N)$ with T_N denoting the transition temperature to an incommensurate helical spin structure, while B is a temperature-independent parameter. The absolute value of c in Eq. (3.3) is required for the invariance under the integral translations, since we have

$$\boldsymbol{t}_n c = c \exp(-i\boldsymbol{k}_1 \cdot \boldsymbol{t}_n). \tag{3.4}$$

This potential is also invariant under the rotational symmetry elements of the group $P3m1'$, represented by the matrices of the irrep Γ_2 in Table, and under the time-reversal operation. The potential in Eq. (3.3) could be supplemented with terms connected with the elastic deformation of the Dy layers. This would lead to a change in the transition temperature. This effect was discussed in Ref. [8] for the b-axis Dy/Y superlattice. Since primarily we are concerned with the determination of the spin structure and the respective cross-section for magnetic neutron scattering, we will not present the respective calculation. The equilibrium value of the coefficient c, corresponding to the minimum value of the thermodynamic potential, is proportional then to the square root of $(T_N - T)$.

The basis function $\Psi(r) = Pf(r)$ is determined by applying the projection operator

$$P = \frac{1}{6} \sum_{R \in C_{3v}} D(R)R, \tag{3.5}$$

where $D(R)$ denote the one-dimensional-matrix elements of the irrep Γ_2 in Table, to the axial-vector trial function in the following form:

$$f(r) = S_0 \begin{pmatrix} \cos(\boldsymbol{Q} \cdot \boldsymbol{r}) + \sum_j p_j(\boldsymbol{a}_j \cdot \boldsymbol{b}_j) \\ \sin(\boldsymbol{Q} \cdot \boldsymbol{r}) + \sum_j q_j(\boldsymbol{a}_j \cdot \boldsymbol{b}_j) \end{pmatrix}, \tag{3.6}$$

where the elements of the column matrix refer to the x and y axes of the Cartesian system of coordinates in Fig. 1, related with the hexagonal system of axes by the equalities between the respective unit vectors

$$\boldsymbol{e}_x = \boldsymbol{e}_1, \quad \boldsymbol{e}_y = (\boldsymbol{e}_1 + 2\boldsymbol{e}_2)/\sqrt{3}, \quad \boldsymbol{e}_z = \boldsymbol{e}_3, \tag{3.7}$$

where S_0 is a real scalar parameter, $\boldsymbol{Q} = \boldsymbol{k}_1,\ \boldsymbol{k}_1 + \boldsymbol{b}_3$, with $|\boldsymbol{b}_3| = 2\pi/c$, where c — the height of the (distorted) Dy crystal unit cell, where $\boldsymbol{a}_1,\ \boldsymbol{a}_2,\ \boldsymbol{a}_3$ are the basis vectors of a Dy crystal and $\boldsymbol{b}_1,\ \boldsymbol{b}_2,\ \boldsymbol{b}_3$ are the respective reciprocal lattice vectors, while p_j and q_j with $j = 1, 2, 3$ are real parameters. From Eq. (3.6), for appropriately chosen relations among the parameters p_j and q_j, we then find the following spin structure formula:

$$\boldsymbol{S}(\boldsymbol{r}) = cPf(\boldsymbol{r}) = cS_0 \begin{pmatrix} \cos(\boldsymbol{Q} \cdot \boldsymbol{r} + \delta) \\ \pm\sin(\boldsymbol{Q} \cdot \boldsymbol{r} + \delta) \end{pmatrix}, \tag{3.8}$$

where δ is a real parameter which determines the initial phase of the spin helix. The $(\pm)$ signs in Eq. (3.8) refer to clockwise- or anticlockwise-turning helix. The two types of spin structures, obtained from Eq. (3.8), connected with $\boldsymbol{Q} = \boldsymbol{k}_1$ or $\boldsymbol{Q} = \boldsymbol{k}_1 + \boldsymbol{b}_3$, are represented in Fig. 2. These two spin structures would correspond to different minimum values of the thermodynamic potential, if they were supplemented with invariants containing space derivatives of the coefficient c. The respective Lifshitz invariant is connected with the Dzyaloshinskii–Moriya relativistic interaction, while the remaining space-derivative-dependent invariants are connected with spatially inhomogeneous exchange interaction. Since the coefficients of all the invariants are phenomenological, the relative position of the minima corresponding to the two spin structures cannot be theoretically established.

We can generalize Eq. (3.8) for the case when a homogeneous magnetic field is applied in the direction parallel to the helical axis, i.e. to the z-axis. The spin structure in Eq. (3.8) then acquires a constant z-component s_z in the field direction, whose magnitude depends on the magnetic field intensity.

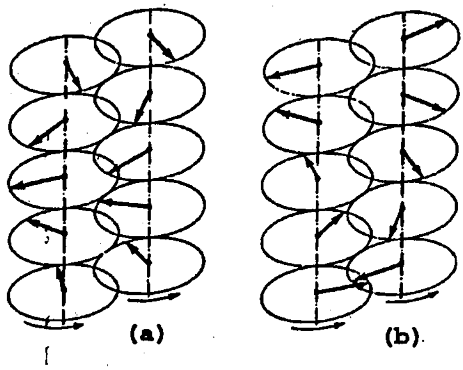

Fig. 2. The mutual orientation of the nearest-neighbour spins in the two types of helical spin structures in Eq. (3.8). Structure (a) corresponds to $\boldsymbol{Q} = \boldsymbol{k}_1$ and structure (b) to $\boldsymbol{Q} = \boldsymbol{k}_1 + \boldsymbol{b}_3$.

4. Cross-section for magnetic scattering of neutrons

We refer to Marshall and Lovesey [9] for magnetic scattering of neutrons. We consider a superlattice with fifteen Dy atomic planes in a Dy/Y bilayer which corresponds to one of the samples in Ref. [1]. The Y-atomic planes are dormant in magnetic scattering. We consider the superlattice in a homogeneous external magnetic field, parallel to the helical axis, when the spins of the helix have a constant z-component. We find that with the accuracy to constant terms, the cross-section for magnetic scattering of neutrons connected with the spin structures in Eq. (3.8), supplemented with the same z-component for all the spins, has the following form:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \propto NS(T)|F(\boldsymbol{\kappa})|^2$$

$$\times \left[m_z^2(1-e_z^2)\sum_{\boldsymbol{K}} E_1\, \delta(\boldsymbol{\kappa}-\boldsymbol{K}) + (1+e_z^2)\sum_{\boldsymbol{K}} E_2 \delta(\boldsymbol{\kappa} \pm \boldsymbol{k}_1 - \boldsymbol{K}) \right], \quad (4.1)$$

where N denotes the number of Dy atoms in the superlattice, $S(T) = c(T)S_0$ is the temperature-dependent spin amplitude, $\boldsymbol{\kappa} = \boldsymbol{q}_0 - \boldsymbol{q}$, where $\boldsymbol{q}_0$ and $\boldsymbol{q}$ are the wave vectors of the incoming and scattered neutrons, respectively, $F(\boldsymbol{\kappa})$ denotes the form factor, e_z is the z-component of the vector $\boldsymbol{e} = \boldsymbol{\kappa}/\kappa$, m_z denotes the directional cosine of the spin vector $\boldsymbol{S}(\boldsymbol{r})$ with the z-direction, while $\boldsymbol{K} = h\boldsymbol{b}_1 + k\boldsymbol{b}_2 + l\boldsymbol{b}_L$, with h, k, l — integers and $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_L$ calculated from Eq. (2.1), is a reciprocal lattice vector. The extinction coefficient E_1 is the same for both the spin structures connected with $\boldsymbol{Q} = \boldsymbol{k}_1$, $\boldsymbol{k}_1 + \boldsymbol{b}_3$, in Eq. (3.8), and is given by

$$E_1 = E_2(\boldsymbol{k}_1), \quad (4.2)$$

where E_2 is connected with $\boldsymbol{Q} = \boldsymbol{k}_1$ in Eq. (3.8) and is given by

$$E_2(k_1) = 15 + 2[13\cos\alpha + 11\cos 4\alpha + 9\cos 6\alpha + 7\cos 8\alpha + 5\cos 10\alpha$$
$$+3\cos 12\alpha + \cos 14\alpha] + 4\cos\beta[7\cos\alpha + 6\cos 3\alpha$$
$$+5\cos 5\alpha + 4\cos 7\alpha + 3\cos 9\alpha + 2\cos 11\alpha + \cos 13\alpha] \quad (4.3)$$

with $\alpha = \pi a_3(\mathrm{Dy})l/L$, $\beta = 2\pi(h-k)/3$. For the second spin structure, connected with $Q = k_1 + b_3$ in Eq. (3.8), the coefficient E_1 is given by Eq. (4.2), while $E_2(k_1 + b_3)$ is obtained from $E_2(k_1)$ in Eq. (4.3) by replacing $\cos\beta$ in the last term in the square bracket by $-\cos\beta$. The coefficients $E_2(k_1)$ and $E_2(k_1 + b_3)$ for $l = 0$, and $(h-k)/3$ — integer, differ by about two orders of magnitude, and can be experimentally distinguished.

5. Conclusion

We have calculated two types of helical spin structures in c-axis Dy/Y superlattice on the assumption that the symmetry of the paramagnetic phase is described by the grey group connected with the resultant crystallographic symmetry group of the superlattice. The comparison of the calculated cross-section for magnetic scattering of neutrons with the experimental data, namely, the existence of magnetic satellite peaks for $h = k = 0$, and $l \neq 0$, indicates that it is the spin structure (a) in Fig. 2 which was revealed by the experiment.

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