Revisit of Dzyaloshinskii-Moriya Interaction with Symmetry

H. Katsumoto[1*], S. Blügel[1]

[1]*Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany*

*h.katsumoto@fz-juelich.de

Introduction

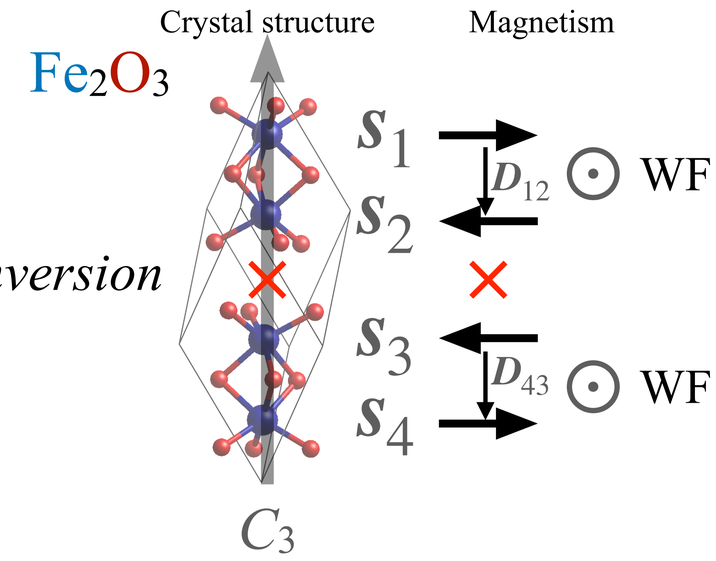
The DMI interaction was described phenomenologically by Dzyaloshinskii [1] and microscopically by Moriya [2] as an explanation for the weak ferromagnetism (WF) due to the effect on SOC in α-Fe_2O_3. However, they do not agree in the argument by *symmetry*. It is questionable whether the two theories are equivalent. In this study, we would like to deepen the discussion of symmetry in α-Fe_2O_3.

Phenomenological by Dzyaloshinskii

$$\Phi = \frac{A}{2}l_1^2 + \frac{B}{2}m^2 + \frac{\alpha}{2}l_{1z}^2 + \frac{b}{2}m_z^2 + \beta(l_{1x}m_y - l_{1y}m_x) + \frac{C}{4}l_1^4$$

Magnetic symmetry-adapted basis

$$\boldsymbol{m} = \boldsymbol{s}_1 + \boldsymbol{s}_2 + \boldsymbol{s}_3 + \boldsymbol{s}_4$$
$$\boldsymbol{l}_1 = \boldsymbol{s}_1 - \boldsymbol{s}_2 - \boldsymbol{s}_3 + \boldsymbol{s}_4$$
$$\boldsymbol{l}_2 = \boldsymbol{s}_1 - \boldsymbol{s}_2 + \boldsymbol{s}_3 - \boldsymbol{s}_4$$
$$\boldsymbol{l}_3 = \boldsymbol{s}_1 + \boldsymbol{s}_2 - \boldsymbol{s}_3 - \boldsymbol{s}_4$$



Microscopic by Moriya

$$\mathcal{H}_{\mathrm{DM}} = -\sum_{<i,j>} \boldsymbol{D}_{ij} \cdot (\boldsymbol{s}_i \times \boldsymbol{s}_j), \quad \boldsymbol{D}_{ij} = -\boldsymbol{D}_{ji}$$

Point group symmetry: $\boldsymbol{D}_{12}, \boldsymbol{D}_{43}$ ∥ 3-fold axis (C_3)

$$\mathcal{H}_{\mathrm{DM}} = -\boldsymbol{D}_{12} \cdot (\boldsymbol{s}_1 \times \boldsymbol{s}_2) - \boldsymbol{D}_{43} \cdot (\boldsymbol{s}_4 \times \boldsymbol{s}_3)$$

Connected by inversion symmetry

Method

Using the *magnetic representation* Γ_{mag} [3], we construct the magnetic structures that serves as a symmetry-adapted basis for the thermodynamic function. This basis is a consequence of the demands on the magnetic structure from the symmetry of the crystal.

$$\Gamma_{\mathrm{mag}} = \Gamma_{\mathrm{perm}} \otimes \Gamma_{\mathrm{axial}}$$

Magnetic Order Ionic Position Classical Spin

I. Representation of ionic position; Γ_{perm}

The space group elements of R-3C

$\{E|0\}\ 2\{C_3|0\}\ 3\{C_2|\tau\}\ \{i|0\}\ 2\{S_6|0\}$
$3\{\sigma_d|\tau\}\ \ \tau = (1/2,1/2,1/2)$

The point group of this space group is D_{3d}.

Wyckoff Position of magnetic ions; 4c

X1; (u, u, u)
X2; (1/2-u, 1/2-u, 1/2-u)
X3; (1/2+u, 1/2+u, 1/2+u)
X4; (1-u, 1-u, 1-u)

Symmetrical operation to leave magnetic-ion position

	E	C_3	C_2	i	S_6	m
X1	X1	X1	X2	X4	X4	X3
X2	X2	X2	X1	X3	X3	X4
X3	X3	X3	X4	X2	X2	X1
X4	X4	X4	X3	X1	X1	X2

Character Table: D_{3d}

	E	C_3	C_2	i	S_6	m
A_{1g}	1	1	1	1	1	1
A_{2g}	1	1	-1	1	1	-1
E_g	2	-1	0	2	-1	0
A_{1u}	1	1	1	-1	-1	-1
A_{2u}	1	1	-1	-1	-1	1
E_u	2	-1	0	-2	1	0

The character table for permutation representation

	E	C_3	C_2	i	S_6	m
Γ_{perm}	4	4	0	0	0	0

×

	E	C_3	C_2	i	S_6	m
Γ_{axial}	3	0	#	#	#	#

=

	E	C_3	C_2	i	S_6	m
Γ_{mag}	12	0	0	0	0	0

II. Representation of axial vector; Γ_{axial}

Find the character table of axial vectors.

$$D_{\mathrm{axial}}(C_3) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

III. Magnetic representation; Γ_{mag}

Reduction to Irreps.

$$\Gamma_{\mathrm{mag}} = A_{1g} + A_{2g} + 2E_g + A_{1u} + A_{2u} + 2E_u$$

Four one-dimensional representation with four kinds
Four two-dimensional representation with two kinds

← Symmetry-adapted basis for Landau theory!

IV. Making site-selective projection operators

$$\hat{P}_{\Gamma_\alpha}^{\mathrm{X}_m(i,j)} = \frac{d_\alpha}{g} \sum_{G \in \mathcal{G}} (\det[D_{\mathrm{vec}}(G)]) \delta_{\mathrm{X}_m, G\mathrm{X}_1} \langle \Gamma_\alpha^i | G | \Gamma_\alpha^j \rangle^* D_{\mathrm{vec}}(G)$$

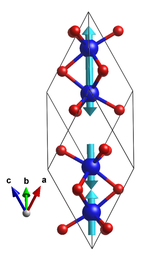
V. Symmetry-adapted basis (Magnetic Structure)

$$\boldsymbol{s}_{\Gamma_\alpha}^{\mathrm{X}_m} = \hat{P}_{\Gamma_\alpha}^{\mathrm{X}_m} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

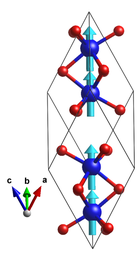
Results and Discussions

One-dimensional irreducible representation (magnetic order)

(Fe_2O_3 State I; *not* WF)

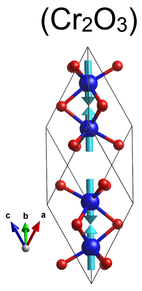


A_{1g} ($\boldsymbol{l}_{1z}$)

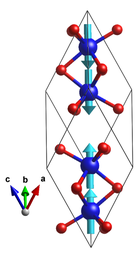


A_{2g} ($\boldsymbol{m}_z$)

(Cr_2O_3)



A_{1u} ($\boldsymbol{l}_{2z}$)

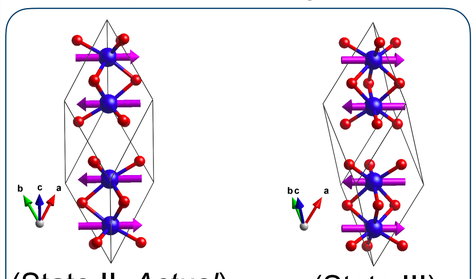


A_{2u} ($\boldsymbol{l}_{3z}$)

Magnetic Inversion

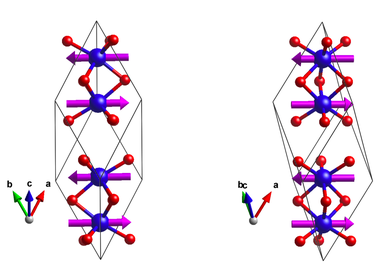
Two-dimensional irreducible representation (magnetic order)

In mirror plane Along two-fold axis In mirror plane Along two-fold axis

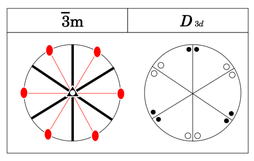


(State II, *Actual*) (State III)

E_g



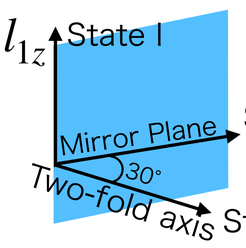
E_u



Magnetic Inversion and WF

$\boldsymbol{m}$ and $\boldsymbol{l}_1$ (x, y-components): E_g
$\boldsymbol{l}_2$ and $\boldsymbol{l}_3$ (x, y-components): E_u

Subgroup and Transition



T: time reversal operator

$\{E|0\}, \{C_3|0\}, \{C_2|\tau\}, \{i|0\}, \{S_6|0\}, \{\sigma_d|\tau\}$ (State I)

subgroup

$\{E|0\}, \{C_2|\tau\}, \{i|0\}, \{\sigma_d|\tau\}$ (State II) × $\{E|0\}, \{C_2T|\tau\}, \{i|0\}, \{\sigma_dT|\tau\}$ (State III)

C_3 symmetry is lost!

Microscopic DMI term

$$\Delta E = -2i\lambda \sum_{n \neq 0} \left(\frac{J(n0,00)\,\langle 0|\boldsymbol{L}_i|n\rangle}{E_{in} - E_{i0}} - \frac{J(0n,00)\,\langle 0|\boldsymbol{L}_j|n\rangle}{E_{jn} - E_{j0}} \right) \cdot (\boldsymbol{s}_i \times \boldsymbol{s}_j)$$

On-site orbital angular momentum

As can be seen from the tabular expression of the D-vector in the above equation, the crystal symmetry is included in the on-site orbital angular momentum.

However, the matrix elements of the orbital angular momentum are the values between the ground state and the excited state, which is difficult to solve analytically. In the present case, Fe^{3+} is d^5 and all the majority states are filled, so the orbital angular momentum of the ground state is not anisotropic. For the microscopic Hamiltonian explanation of the phase transition, a higher order term of the spin interaction would be necessary.

Summary and References

The noncollinear magnetism of Fe_2O_3 is explained by the D-vector, which is defined by the C_3 symmetry, but is lost in the basic magnetic structure showing weak ferromagnetism. Moriya's formula is valid for the microscopic canting state of magnetism, but the two sides do not agree on the symmetry. In addition, without considering the hybridization of ligand oxygen and iron, it is generally impossible to distinguish the magnetic structures of State II and State III only from Moriya's rules, since this is controlled by Heisenberg exchange, and it is not possible to discuss the phase transition between the magnetic structures. On the other hand, the thermodynamic function using the symmetry-adapted magnetic structure as a basis allows us to discuss the phase transition between magnetic structures from their symmetry.

[1] I.E. Dzialoshinskii, *Soviet Physics JETP* **5**, 1259 (1957). [2] T. Moriya, *Physical Review Letters* **4**, 228 (1960). [3] J. Kishine, *Solid State Physics* **45**, 771 (2010)