01,05

Symmetry analysis of conductive antiferromagnetic materials CuMnAs, Mn_2Au

© A.K. Zvezdin[1,2], Z.V. Gareeva[3]

[1] Prokhorov Institute of General Physics, Russian Academy of Sciences, Moscow, Russia
[2] New spintronic technologies, Skolkovo, Moscow, Russia
[3] Institute of Molecule and Crystal Physics, Subdivision of the Ufa Federal Research Centre of the Russian Academy of Sciences, Ufa, Russia

E-mail: zukhragzv@yandex.ru, zvezdin.ak@phystech.edu

Received April 18, 2024
Revised April 18, 2024
Accepted May 8, 2024

Magnetic structures and their interaction with spin-polarized currents in conducting antiferromagnets are considered using the example of CuMnAs and Mn_2Au. Within the framework of the group theoretical approach, a classification of the magnetic order parameters of these crystals was carried out according to the irreducible representations of the space symmetry groups D_{4h}^{7} and D_{4h}^{17}. Invariant combinations of order parameters are obtained that determine the energy of interaction of spin currents with the antiferromagnetism vector.

Keywords: conducting antiferromagnets, electric current, spin current, symmetry.

DOI: 10.61011/PSS.2024.06.58685.42HH

1. Introduction

In recent years, the concept of antiferromagnetic spintronics has seen active development [1–3], due to the potential of using the advantages of antiferromagnetically ordered materials in modern technologies The stability of antiferromagnets to the action of an external magnetic field, high-speed magnetization dynamics and good transport properties make these materials attractive for application in random access memory devices, including the application as components of spin-tunnel magnetoresistive elements [4,5]. The antiparallel orientation of spins in antiferromagnets is responsible for (i) the absence of scattering fields in them as a result of compensation for the resulting magnetization of the crystal; (ii) the occurrence of a pair of torques resulting in high frequencies of magnetization precession; high speeds of movement of magnetic domain boundaries and other technologically important effects.

The variety of electrical properties also ensures the multifunctionality of antiferromagnetics. Classical antiferromagnetics — oxides with antiferromagnetic (AFM) spin ordering are mostly dielectrics; in technological terms, AFM multiferroic oxides are relevant, promising for applying in energy-saving devices and technologies. The AFM semimetals and conductors, CuMnAs, Mn_2Au, Mn_3Sn, Mn_3Ge, Mn_3Pt, are attracting an increasing attention of researchers, mainly because the magnetic state in them can be switched under the impact of electric and spin-polarized currents; the effect of giant magnetoresistance is realized; there are additional rotational moments that participate in the spin transfer effect; the anomalous Hall effect features can be observed which are not present in most AFM. A series of theoretical and experimental works 2016−2019 covers the study of the nature of these effects [4–12].

Conducting antiferromagnetics offer interesting prospects for technological applications in spintronics. We will limit ourselves in this paper to the range of issues associated with the impact of electric and spin currents on the magnetic structure of conducting antiferromagnetics, which is a relevant aspect for the realization of antiferromagnetic multilevel memory [13]. To be definite, let us review the antiferromagnetics CuMnAs and Mn_2Au, the electronic structure, magnetic and transport properties of which have been actively studied during the recent years [5,6,14,15] in connection with the studies of high-speed dynamics of domain boundaries [7,16].

The goal of this work is to study the opportunities of optimizing magnetoresistance effects in spin-tunneling devices where a conductive antiferromagnet is applied as a free magnetic layer. To solve this problem, it is necessary to study the magnetic states that can be implemented in a free layer of an antiferromagnetic under the impact of a spin current, for example, through a tunnel contact separating the polarizer layer and the free layer of a magnetoresistance device. Let us determine the magnetic configurations realized in antiferromagnetics of tetragonal symmetry using the methods of theory group analysis and

analyze the effects related to the action of charge and spin currents.

2. Spin currents. Problem formulation

The problem of magnetic states in an antiferromagnet occurring due to the action of spin-polarized currents can be solved using the Lagrangian formalism technique, the Lagrange function and the Rayleigh dissipative function have the form [17,18]

$$L = \chi_\perp \dot{\boldsymbol{l}}/2\gamma^2 - \chi_\perp \boldsymbol{H}\left[\boldsymbol{l}\times\dot{\boldsymbol{l}}\right]/\gamma - \Phi - W,$$

$$R = \alpha M_0 \dot{\boldsymbol{l}}^2/2\gamma, \qquad (1)$$

where γ — gyromagnetic ratio, α — dissipation parameter, $\boldsymbol{l}$ — unit vector of antiferromagnetism, Φ — thermodynamic potential of the system, W — energy density associated with torques acting from spin-polarized currents.

Spin-polarized currents are currents related to spin transfer processes are determined by relations of the form

$$\boldsymbol{j}_\sigma = \sum_i \boldsymbol{V}_i \otimes \boldsymbol{s}_i, \quad |\boldsymbol{j}_\sigma| = p\frac{\hbar s}{e} J, \qquad (2)$$

where $p = (N_+ - N_-)/(N_+ + N_-)$ — spin polarization, $N_\mp$ — number of electrons with spin $s = \mp 1/2$.

The peculiarity of spin currents from the point of view of symmetry is that the spin current does not change the sign in case of the time inversion, however it changes the sign in case of spatial inversion like the electric current ($z \to -z$, $y \to -y$, $x \to -x$). Spin currents can be of two types: (i) injection currents j^s_{ij}, used in spintronics in multilayer nanostructures in experiments such as STT (due to the angular momentum transfer effect) or spin-Hall effects, (ii) spin currents, as part of the spin-polarized current arising in magnetic-ordered materials according to Mott's idea. In this case, the charging current can arise due to external potential differences, temperature gradients and concentration gradients. An example is spin currents caused by the Seebeck effect

$$\boldsymbol{J}^T_s = -\frac{\hbar}{2e}\sigma\nabla T,$$

σ — Seebeck coefficient [19].

3. Magnetic structure of conducting antiferromagnetics. CuMnAs, Mn_2Au

Let us review the crystal structure and magnetic properties of antiferromagnetics CuMnAs and Mn_2Au. The lattice cells of CuMnAs and Mn_2Au crystals contain four CuMnAs and Mn_2Au molecules; the crystal structures of CuMnAs and Mn_2Au are described by space symmetry groups D^7_{4h} and D^{17}_{4h}, respectively. In both cases, the Mn^{3+} ions occupy positions 4*c* in the Wyckoff notation.

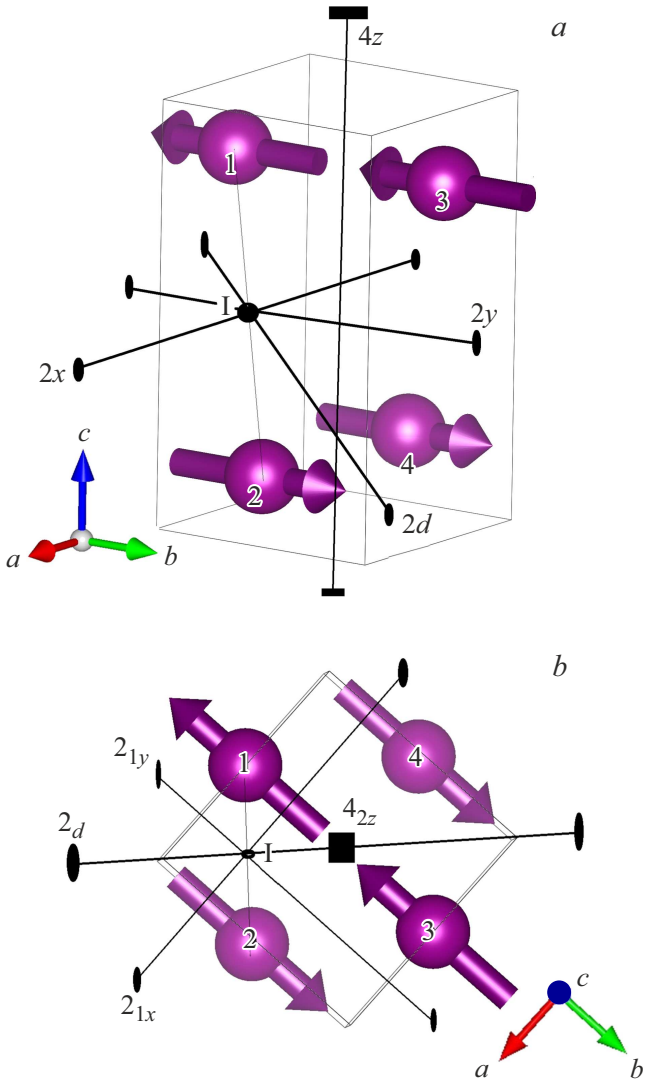

Figure 1. *a* — lattice cell CuMnAs; *b* — projection of the cell onto the plane *ab*, position of the main symmetry elements.

Groups D^7_{4h} and D^{17}_{4h} contain a set of 16 symmetry operations, from which independent elements $4^+_{2z}, 2_d, \bar{1}$ can be selected as group oscillators. Further, let us review the CuMnAs antiferromagnetic for the illustration and the results obtained will also be valid for Mn_2Au due to the symmetry.

The location of symmetry elements — second-order helical axes $2_{1y}, 2_{1y}$, fourth-order helical axis 4^+_{2z}, second-order axis $2d$ and inversion $\bar{1}$ in the CuMnAs lattice cell, as well as on its projection onto the plane perpendicular to the main axis of the crystal 4^+_{2z}, shown in the Figure 1. Mn^{2+} ions occupy double positions $2c\{4mm\}$ with coordinates: $(0, 1/2, z) = (0, 0.50, 0.16402)$.

The nature of magnetic ordering is associated with the crystal structure. Mn^{3+} ions in CuMnAs form an antiferromagnetic ordered ***G***-type structure at temperatures of $T = 330-360$ K according to neutron diffraction data [20]. Let us introduce the basis vectors of magnetic sublattices as

Table 1. Permutation transformations of Mn^{3+} ions and basis vectors under the impact of group generators G_F

G_F	1	2	3	4	G_F	F	A	G	C
$\bar{1}$	2	1	4	3	$\bar{1}$	F	$-A$	$-G$	C
4^+_{2z}	4	3	2	1	4^+_{2z}	F	$-A$	$-G$	$-C$
2_d	2	1	4	3	2_d	F	$-A$	$-G$	C

magnetic order parameters

$$\begin{aligned} \boldsymbol{F} &= \boldsymbol{\mu}_1 + \boldsymbol{\mu}_2 + \boldsymbol{\mu}_3 + \boldsymbol{\mu}_4, \\ \boldsymbol{A} &= \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2 - \boldsymbol{\mu}_3 + \boldsymbol{\mu}_4, \\ \boldsymbol{G} &= \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2 + \boldsymbol{\mu}_3 - \boldsymbol{\mu}_4, \\ \boldsymbol{C} &= \boldsymbol{\mu}_1 + \boldsymbol{\mu}_2 - \boldsymbol{\mu}_3 - \boldsymbol{\mu}_4. \end{aligned} \tag{3}$$

Since the magnetic moments of the ions are identical in magnitude, $|\boldsymbol{\mu}_1| = |\boldsymbol{\mu}_2| = |\boldsymbol{\mu}_3| = |\boldsymbol{\mu}_4|$, $\boldsymbol{\mu}_1 \uparrow\uparrow \boldsymbol{\mu}_3$, $\boldsymbol{\mu}_2 \uparrow\uparrow \boldsymbol{\mu}_4$, $\boldsymbol{\mu}_1 \uparrow\downarrow \boldsymbol{\mu}_2$, $\boldsymbol{\mu}_3 \uparrow\downarrow \boldsymbol{\mu}_4$, it is convenient to proceed to the approximation of a two-sublattice magnet

$$\boldsymbol{M} = \frac{1}{2M_0}(\boldsymbol{M}_1 + \boldsymbol{M}_2), \quad \boldsymbol{L} = \frac{1}{2M_0}(\boldsymbol{M}_1 - \boldsymbol{M}_2), \tag{4}$$

where M_0 — the sublattice magnetization value, $\boldsymbol{M}_1 = \boldsymbol{\mu}_1 + \boldsymbol{\mu}_3$, $\boldsymbol{M}_2 = \boldsymbol{\mu}_2 + \boldsymbol{\mu}_4$.

Let us make up a position code from the generators of the group, specifying the permutation properties of the ions in accordance with the Figure 1

$$\bar{1}\begin{pmatrix}1-2\\3-4\end{pmatrix} 4^+_{2z}\begin{pmatrix}1-4\\2-4\end{pmatrix} 2_d\begin{pmatrix}1-2\\3-4\end{pmatrix}.$$

Table 1 shows how the positions of ions are transformed and the basis vectors are transformed under the impact of generators of the group D^7_{4h}.

Let us obtain the code (Turov indices) for the AFM vector $\boldsymbol{G}$ using Table 1:

$$\bar{1}(-)4^+_{2z}(-)2_d(-). \tag{5}$$

Let us classify the ferro- and antiferromagnetism vectors ($\boldsymbol{M}$ and $\boldsymbol{L}$) using code (5) which are parameters of the magnetic ordering of CuMnAs, as well as the components of the spin ($\boldsymbol{J}_s$) and charge currents ($\boldsymbol{J}$) according to the irreducible representations of the crystal symmetry group (Table 2). Let us note that the indices i and j in the spin current tensor j^s_{ij} are associated with the components of electric current J_i and magnetization M_j, while the action of the symmetry operations 4^+_{2z} and 2_d is such that $j^s_{ij} = j^s_{ji}$.

Γ_i $(i = 1{-}10)$ as basis functions for irreducible representations in various situations can be taken as even and odd quantities with respect to time inversion, for example, $\boldsymbol{J}$ and $\boldsymbol{E}$. We believe that such a dichotomy will not cause difficulties for the reader depending on the specific physical situation.

Let us consider the interaction of spin currents with the components of the antiferromagnetic vector $\boldsymbol{L}$. The following expressions for the energy of interaction of spin currents with the components of the vector $\boldsymbol{L}$ can be obtained from Table 2, using the operations of multiplication of irreducible representations

$$\begin{aligned} W = {} & a_1(J^s_{xz}L_y + J^s_{yz}L_x) + a_2(J^s_{zx}L_y + J^s_{yz}L_x) \\ & + a_3(J^s_{xy}L_z + J^s_{yz}L_x) + a_4(J^s_{xx} - J^s_{yy})H_zL_z. \end{aligned} \tag{6}$$

Table 2. Irreducible representations (IR) of the group D^7_{4h} and basis functions

	$\bar{1}$	4^+_{2z}	2_d	M_i, L_i	J^s_{ij}
Γ_1	1	1	1	$L_x^2 + L_y^2$	
Γ_2	1	1	−1	M_z, H_z	
Γ_3	−1	−1	1	L_z	$j^s_{xy} + j^s_{yx}$
Γ_4	−1	1	−1	J_z, E_z	
Γ_5	−1	1	1		j^s_{zz}, $j^s_{xx} + j^s_{yy}$
Γ_6	−1	−1	−1	M_zL_z	$j^s_{xx} - j^z_{yy}$
Γ_7	1	−1	1	$M_zL_zJ_z$	
Γ_8	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}M_x\\M_y\end{pmatrix}, \begin{pmatrix}H_x\\H_y\end{pmatrix}$	
Γ_9	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$	$\begin{pmatrix}L_x\\L_y\end{pmatrix}$	
Γ_{10}	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix}$	$\begin{pmatrix}J_x\\J_y\end{pmatrix}, \begin{pmatrix}E_x\\E_y\end{pmatrix}$	
Γ_{11}	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}0&1\\-1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$		$\begin{pmatrix}J^s_{zx}\\J^s_{zy}\end{pmatrix}$

A quadratic form composed of vector components $\boldsymbol{L, M, H, E}$ is needed to study spin dynamics, which determines the total thermodynamic potential of the system, which includes exchange energy, anisotropy energy, Zeeman energy and magnetoelectric energy. It can also be composed using Table 2.

$$\Phi = a\boldsymbol{M}^2 + c_1(L_x^2 + L_y^2) + c_2 L_z^2 + d(\boldsymbol{M}\cdot\boldsymbol{L})^2 + g_1 L_z(M_x E_y + M_y E_x) + g_2 M_z(L_x E_y + L_y E_x) + g_3 E_z(L_y M_x + L_x M_y). \quad (7)$$

An expression of the form (6) can be considered as a component of the general theory (diagram) for studying the physical properties of antiferromagnetics, developed by Soviet scientists Dzyaloshinski, Borovik-Romanov, Turov [21–27] (see also Chapter 14 in [27]), based on the use of space symmetry groups of crystals. This diagram, i.e. formulas (1), (6), (7) can be used to analyze the spin dynamics of conducting antiferromagnets, which has been widely studied in recent years.

Until now, the observed singularities of the dynamics of the antiferromagnetic spin systems CuMnAs and Mn_2Au [4–8,12,16] were explained as part of the concept of NSOT — Neel spin orbital torque, obtained by the authors of the papers [6,8,12,16] based on microscopic consideration.

The approach presented in this paper allows studying the spin dynamics of conducting antiferromagnets from a more general position, since it is based on the use of the spatial symmetry of these materials. We believe that this approach could be a useful complement to the pioneering work mentioned above. We do not aim to fully develop this theory in this short report. We only point out that, using the quadratic form of the thermodynamic potential considered above and substituting it into the Lagrangian of system (1) taking into account (6) and (7), we obtain a complete diagram for describing the spin dynamics of conducting antiferromagnetics as part of the symmetry approach.

Funding

The study was supported by the grant of the Ministry of Science and Education of the Russian Federation. Agreement No. 075-11-2022-046.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] V. Baltz, A. Manchon, M. Tsoi, T. Moriyama, T. Ono, Y. Tserkovnyak. Rev. Mod. Phys. **90**, 015005 (2018).
[2] T. Jungwirth, X. Marti, P. Wadley, J. Wunderlich. Nature Nanotech. **11**, 3 (2016).
[3] O. Gomonay, T. Jungwirth, J. Sinova. Phys. Status Solidi — Rapid Res. Lett. **11**, 1700022 (2017).
[4] P. Wadley, S. Reimers, M.J. Grzybowski, C. Andrews, M. Wang, J.S. Chauhan, B.L. Gallagher, R.P. Campion, K.W. Edmonds, S.S. Dhesi, F. Maccherozzi, V. Novak, J. Wunderlich, T. Jungwirth. Nature Nanotech. **13**, 362 (2018).
[5] P. Wadley, B. Howells,J. Zelezný, C. Andrews, V. Hills, R.P. Campion, V. Novák, K. Olejník, F. Maccherozzi, S.S. Dhesi, S.Y. Martin, T. Wagner, J. Wunderlich, F. Freimuth, Y. Mokrousov, J. Kuneš, J.S. Chauhan, M.J. Grzybowski, A.W. Rushforth, K.W. Edmonds, B.L. Gallagher, T. Jungwirth. Science **351**, 587 (2016).
[6] J. Godinho, H. Reichlová, D. Kriegner, V. Novák, K. Olejník, Z. Kašpar, Z. Šobáň, P. Wadley, R.P. Campion, R.M. Otxoa, P.E. Roy, J. Železný, T. Jungwirth, J. Wunderlich. Nature Commun. **9**, 4686 (2018).
[7] M.J. Grzybowski, P. Wadley, K.-W. Edmonds, R. Beardsley, V. Hills, R.-P. Campion, B.-L. Gallagher, J.-S. Chauhan, V. Novak, T. Jungwirth, F. Maccherozzi, S.-S. Dhes. Phys. Rev. Lett. **118**, 057701 (2017).
[8] L. Baldrati, O. Gomonay, A. Ross, M. Filianina, R. Lebrun, R. Ramos, C. Leveille, F. Fuhrmann, T.-R. Forrest, F. Maccherozzi, S. Valencia, F. Kronast, E. Saitoh, J. Sinova, M. Kläui. Phys. Rev. Lett. **123**, 177201 (2019).
[9] A. Manchon, J. Železný, I.M. Miron, T. Jungwirth, J. Sinova, A. Thiaville, K. Garello, P. Gambardella. Rev. Mod. Phys. **91**, 035004 (2019).
[10] T. Shiino, S.-H. Oh, P.M. Haney, S.-W. Lee, G. Go, B.-G. Park, K.-J. Lee. Phys. Rev. Lett. **117**, 087203 (2016).
[11] H. Van den Berg, W. Clemens, G. Gieres, G. Rupp, W. Schelter, M. Vieth. IEEE Transact. Magn. **32**, 4624 (1996).
[12] O. Gomonay, T. Jungwirth, J. Sinova. Phys. Rev. Lett. **117**, 017202 (2016).
[13] K. Olejník, V. Schuler, X. Marti, V. Novák, Z. Kašpar, P. Wadley, R.P. Campion, K.W. Edmonds, B.L. Gallagher, J. Garces, M. Baumgartner, P. Gambardella, T. Jungwirth. Nature Commun. **8**, 1 (2017).
[14] P. Wadley, V. Novák, R.P. Campion, C. Rinaldi, X. Martí, H. Reichlová, J. Železný, J. Gazquez, M.A. Roldan, M. Varela, D. Khalyavin, S. Langridge, D. Kriegner, F. Máca, J. Mašek, R. Bertacco, V. Holý, A.W. Rushforth, K.W. Edmonds, B.L. Gallagher, C.T. Foxon, J. Wunderlich, T. Jungwirth. Nature Commun. **4**, 1 (2013).
[15] J. Volný, D. Wagenknecht, J. Železný, P. Harcuba, E. Duverger-Nedellec, R.H. Colman, J. Kudrnovský, I. Turek, K. Uhlířová, K. Výborný. Phys. Rev. Mater. **4**, 064403 (2020).
[16] J. Železný, P. Wadley, K. Olejn´ k, A. Hoffmann, H. Ohno. Nature Phys. **14**, 3 (2018).
[17] A.F. Andreev, V.I. Marchenko. Uspekhi fizicheskikh nauk **130**, *1*, 39 (1980). (in Russian).
[18] A.K. Zvezdin, A.A. Mukhin, Kratkiye soobshch. po fizike, FIAN **12**, 10 (1981). (in Russian).
[19] K. Uchida, S. Takahashi, K. Harii, J. Ieda, W. Koshibae, K. Ando, S. Maekawa, E. Saitoh. Nature **455**, 7214 (2008).
[20] J. Mündelein, H.-U. Schuster. Z. Naturforschung B **47**, 925 (1992).
[21] E.A. Turov, V.V. Nikolaev. UFN **175**, 457 (2005). (in Russian).
[22] I.E. Dzyaloshinski. ZhETF **46**, 1420 (1964). (in Russian).
[23] I.E. Dzyaloshinski. ZhETF **19**, 960 (1964). (in Russian).
[24] I.E. Dzyaloshinski. ZhETF **20**, 223 (1965). (in Russian).

[25] A.S. Borovik-Romanov. Lektsii po nizkotemperaturnomu magnetizmu. In-t fiz. problem im. P.L. Kapitsy RAN, M. (2010). 55 s. (in Russian).
[26] E.A. Turov, A.V. Kolchanov, V.V. Menshenin, I.F. Mirsaev, V.V. Nikolaev. Symmetriya i fizicheskiye svoystva antiferromagnetikov. Fizmatlit, M. (2001). 559 s. (in Russian).
[27] A.K. Zvezdin, V.M. Matveev, A.A. Mukhin, A.I. Popov. Redkozemelnyie iony v magnitouporyadochennykh kristallakh. Nauka, M. (1985). 295 s. (in Russian).

Translated by A.Akhtyamov