### MAGNETIC POINT GROUP SYMMETRIES OF SPONTANEOUSLY POLARIZED AND/OR MAGNETIZED DOMAIN WALLS

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We present a list of the 125 magnetic point groups associated with possible layer groups of domain walls. For each group we give the direction of the spontaneous polarization and/or magnetization allowed by the magnetic point group symmetry.

*Keywords*: domain walls, domain wall symmetry, spontaneously polarized domain walls, spontaneously magnetized domain walls

#### INTRODUCTION

The existence of spontaneous polarization in domain walls was predicted in several particular cases, e.g. in quartz<sup>[1]</sup> and in magnetoelectric  $Cr_2O_3$  crystals<sup>[2]</sup>. The appearance of spontaneous polarization in domain walls was studied systematically in magnetically ordered crystals<sup>[3]</sup> and symmetry predictions of spontaneous polarization and/or magnetization in domain walls were obtained for all non-ferroelastic domain walls<sup>[4,5]</sup>. It was shown that all ferroelastic domain walls have polar symmetry and can, therefore, carry spontaneous polarization<sup>[6]</sup>.

As the appearance of a spontaneous polarization and/or spontaneous magnetization in homogeneous crystals depends of the crystal's symmetry, the appearance of these spontaneous quantities in domain

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walls depends on the domain wall's symmetry. Since domain walls can be considered as thin layers, their symmetry is described by one of the 528 classes of magnetic layer groups <sup>[7,8]</sup>. In the continuum (continuous medium) approximation, to determine the layer's physical properties, the discrete translations of the layer group symmetry are replaced by a group of two-dimensional continuous translations. Such groups have been named *point-like* layer groups<sup>[9]</sup>. Since the physical properties are invariant under translations, it is the magnetic point group of the magnetic layer group which determines the domain wall's physical properties, e.g. the domain wall's spontaneous polarization and magnetization.

Holser<sup>[10]</sup> has listed 31 point groups associated with non-magnetic layer groups. Magnetic point groups associated with magnetic layer groups have been derived<sup>[2]</sup>, from where it follows that there are 125 classes of such groups. We divide these classes into four groupings:

- (1) Magnetic point groups which allow both a non-zero electric polarization and a non-zero magnetic moment.
- (2) Magnetic point groups which allow a non-zero electric polarization but require a zero magnetic moment.
- (3) Magnetic point groups which allow a non-zero magnetic moment but require a zero electric polarization.
- (4) Magnetic point groups which require both a zero electric polarization and a zero magnetic moment.

The magnetic point groups of these four classes are given, respectively, in Tables 1 through 4. The x and y rectangular coordinates are assumed to be in the plane of the domain wall, and the z coordinate perpendicular to the plane. Magnetic point groups, given in the first column, are followed by the components of the polarization P and magnetization P. For the cases where the magnetic point groups allow both a non-zero polarization and non-zero magnetization additional information is given on the right related to the orientation of the polarization and magnetization with respect to each other and relative to the normal of the planar domain wall.

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From these tables we see that in most cases the domain wall's magnetic point group symmetry uniquely determines the direction of the spontaneous polarization and/or magnetization. In a few cases the direction is partially determined, e.g. for the magnetic point group  $m_X'$  we have  $\mathbf{P} = (0, P_Y, P_Z)$  and  $\mathbf{M} = (0, M_Y, M_Z)$ . Only in the case of the identity magnetic point group symmetry is the direction of both the spontaneous polarization and magnetization arbitrary.

These tables give the possible spontaneous polarizations and magnetizations which can arise in a domain wall and can be used in determining physical properties which arise in a domain wall.

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Table 1: Magnetic point groups which allow both a non-zero polarization and non-zero magnetization

Magnetic Point Group	Polarization Magnetization	
$2_{\rm X}$ $m_{\rm Z}'m_{\rm Y}'2_{\rm X}$	$P = (P_X, 0, 0) M = (M_X, 0, 0)$	<b>P</b> parallel to <b>M</b> , both perpendicular to normal
$m_Z'm_X^{}2_Y'$	$P = (0, P_Y, 0)$ $M = (M_X, 0, 0)$ $P$ poboth norm	perpendicular to
$m_Z$ '	$P = (P_X, P_Y, 0) M = (M_X, M_Y, 0)$	<b>P</b> , <b>M</b> arbitrary angle, both perpendicular to normal
$\begin{array}{ccc} 2_Z & m_X' m_{Y}' 2_Z \\ 4_Z & 4_Z m_{X}' m_{XY}' \\ 3_Z & 3_Z m_{X}' \\ 6_Z & 6_Z m_{X}' m_{Y}' \end{array}$	$P = (0, 0, P_Z) M = (0, 0, M_Z)$	<b>P</b> parallel to <b>M</b> , both parallel to normal
$m_X'm_Y2_Z'$	$P = (0, 0, P_Z) M = (0, M_Y, 0)$	<b>P</b> parallel to, and <b>M</b> perpendicular to normal
2 <sub>z</sub> '	$P = (0, 0, P_Z) M = (M_X, M_Y, 0)$	<b>P</b> parallel to, and <b>M</b> perpendicular to normal
$m_Z m_X' 2_Y'$	$P = (0, P_Y, 0) M = (0, 0, M_Z)$	<b>P</b> perpendicular to, and <b>M</b> parallel to normal
$m_Z$	$P = (P_X, P_Y, 0) M = (0, 0, M_Z)$	<b>P</b> perpendicular to, and <b>M</b> parallel to normal
2 <sub>x</sub> '	$P = (P_X, 0, 0)  M = (0, M_Y, M_Z)$	<b>P</b> perpendicular to, and <b>M</b> in plane containing normal
$m_{\chi}$	$P = (0, P_Y, P_Z) M = (M_X, 0, 0)$	<b>P</b> in plane containing normal, and <b>M</b> perpendicular to normal
$m_X$	$P = (0, P_Y, P_Z) M = (0, M_Y, M_Z)$	<b>P</b> and <b>M</b> in same plane containing

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normal

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$$P = (P_X, P_Y, P_Z) M = (M_X, M_Y, M_Z)$$

Table 2: Magnetic point groups which allow both a non-zero magnetization and require a zero polarization

Magnetic P	oint Group		Polarization Magnetization
$2_{\rm X}/{\rm m}_{\rm X}$	$2_{\rm X}2_{\rm Y}'2_{\rm Z}'$	$m_X m_Y ' m_Z '$	$P = (0, 0, 0)$ $M = (M_X, 0, 0)$
$2_{\rm Z}/m_{\rm Z}$	$2_{x}'2_{y}'2_{z}$	$m_X'm_Y'm_Z$	$\overline{4}_Z$ $P = (0, 0, 0)$ $M = (0, 0, M_Z)$
$4_{\rm Z}/m_{\rm Z}$	$4_z 2_x 2_x $	$\overline{4}_{z}2_{x}'m_{xy}'$	$4_{\rm Z}/m_{\rm Z}m_{\rm X}'m_{\rm XY}'$
$\overline{3}_{z}$	$3_{\rm Z}2_{\rm X}$	$\overline{3}_{Z}m_{X}'$	$\overline{6}_{Z}$
$6_{\rm Z}/m_{\rm Z}$	$6_Z 2_X' 2_Y'$	$\overline{6}_Z m_X' 2_Y'$	$6_{\rm Z}/{\rm m_{\rm Z}m_{\rm X}'{\rm m_{\rm Y}}'}$
2 <sub>Z</sub> '/m <sub>Z</sub> '			$P = (0, 0, 0)$ $M = (M_X, M_Y, 0)$
$2_{\rm X}'/m_{\rm X}'$			$P = (0, 0, 0)$ $M = (0, M_Y, M_Z)$
<u>1</u>			$P = (0, 0, 0)  M = (M_X, M_Y, M_Z)$

Table 3: Magnetic point groups which allow a non-zero polarization and require a zero magnetization

Magneatic Point Group		Group	Polarization Magnetization
2 <sub>x</sub> 1'	$m_z m_y 2_x$	$m_z m_y 2_x 1'$	$P = (P_X, 0, 0)$ $M = (0, 0, 0)$
2 <sub>z</sub> 1'	$m_X m_Y 2_Z$	$m_X m_Y 2_Z 1'$	$4_{z}1'$ $P = (0, 0, P_{z}) M = (0, 0, 0)$
4 <sub>z</sub> '	$4_{Z}m_{X}m_{XY} \\$	$4_Z m_X m_{XY} 1'$	$4_{\rm Z}'m_{\rm X}m_{\rm XY}'$
3 <sub>z</sub> 1'	$3_{Z}m_{X}$	$3_Z m_X 1'$	6 <sub>z</sub> 1'
6 <sub>z</sub> '	$6_{\rm Z} m_{\rm X} m_{\rm Y}$	$6_{\rm Z}$ $m_{\rm X}$ $m_{\rm Y}$ 1'	$6_{\rm Z}'m_{\rm X}m_{\rm Y}'$
m <sub>z</sub> 1'			$P = (P_X, P_Y, 0)  M = (0, 0, 0)$
m <sub>x</sub> 1'			$P = (0, P_Y, P_Z)  M = (0, 0, 0)$
11'			$P = (P_X, P_Y, P_Z) M = (0, 0, 0)$

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Table 4: Magnetic point groups which require both a zero polarization and zero magnetization

Magnetic Point Group			Polarization	Magnetization	
<u>1</u> 1'	<u>1</u> '	$2_{\rm Z}/{\rm m_{\rm Z}}1'$	$2_{\rm Z}/{\rm m_{\rm Z}}'$	$\mathbf{P} = (0, 0, 0)$	$\mathbf{M} = (0, 0, 0)$
2 <sub>Z</sub> '/m <sub>Z</sub>	$2_{\rm X}/m_{\rm X}1'$	$2_{\rm X}/{\rm m_{\rm X}}'$	$2_{\rm X}'/m_{\rm X}$		
$2_{x}2_{y}2_{z}$	$2_{\mathrm{X}}2_{\mathrm{Y}}2_{\mathrm{Z}}1'$	$m_X m_Y m_Z$	$m_X m_Y m_Y$	n <sub>z</sub> 1'	
$m_X'm_Y'm_Z'$	$m_X m_Y m_Z'$	$m_X' m_Y m_Z$	$\overline{4}_{z}1'$		
4 <sub>z</sub> '	$4_z/m_z1'$	$4_{\rm Z}'/m_{\rm Z}$	$4_{\rm Z}/{\rm m_{\rm Z}}'$		
$4_{z'}/m_{z'}$ $4_{z}2_{x}2_{xy}$ $4_{z}2_{x}2_{xy}1'$ $4_{z'}2_{x}2_{xy}'$					
$\overline{4}_{Z}2_{X}m_{XY}$	$\overline{4}_{z}2_{x}m_{xy}1'$	$\overline{4}_{z}'2_{x}m_{xy}'$	$\overline{4}_{z}'2_{x}'n$	$\mathbf{n}_{\mathrm{XY}}$	
$4_{Z}/m_{Z}m_{X}m_{XY} \qquad \qquad 4_{Z}/m_{Z}m_{X}m_{XY}1'$		.1'			
$4_{\rm Z}'/m_{\rm Z}m_{\rm X}m_{\rm XY}'$		$4_{\rm Z}/{\rm m_{\rm Z}}'{\rm m_{\rm X}}'{\rm m_{\rm XY}}'$			
$4_{\mathrm{Z}}/\mathrm{m_{\mathrm{Z}}}\mathrm{m_{\mathrm{X}}}\mathrm{m_{\mathrm{XY}}}$ $4_{\mathrm{Z}}^{\mathrm{I}}/\mathrm{m_{\mathrm{Z}}}\mathrm{m_{\mathrm{X}}}\mathrm{m_{\mathrm{XY}}}$		Y '			
$\overline{3}_{z}1'$	$\overline{3}_{z'}$	$3_z 2_x$	$3_z 2_x 1'$		
$\overline{3}_{Z}m_{X}$	$\overline{3}_{Z}m_{X}1'$	$\overline{3}_{z}$ 'm $_{x}$ '	$\overline{3}_{z}$ 'm <sub>x</sub>		
$\overline{6}_{z}1'$	$\overline{6}_{z}'$	$6_{\rm Z}/m_{\rm Z}1'$	6 <sub>z</sub> '/m <sub>z</sub> '		
$6_{\rm Z}/{\rm m_{\rm Z}}'$	$6_{\rm Z}'/{\rm m}_{\rm Z}$	$6_{\rm Z}2_{\rm X}2_{\rm Y}$	$6_z 2_x 2_y$	1'	
$6_z'2_x2_y'$	$\overline{6}_{z}m_{x}2_{y}$ $\overline{6}_{z}$	$m_X 2_Y 1'$	$\overline{6}_{z}$ 'm <sub>x</sub> '2 <sub>y</sub>		
$\overline{6}_{z}$ 'm <sub>x</sub> 2 <sub>y</sub> '	$6_{\rm Z}/m_{\rm Z}m_{\rm X}m_{\rm Y}$	$6_{\rm Z}/{\rm m_{\rm Z}m_{\rm X}m_{\rm Y}}$	1' 6 <sub>z</sub> '/m <sub>z</sub> 'r	$m_X m_Y'$	
$6_{\mathrm{Z}}/\mathrm{m_{\mathrm{Z}}'m_{\mathrm{X}}'m_{\mathrm{Y}}'}$ $6_{\mathrm{Z}}/\mathrm{m_{\mathrm{Z}}'m_{\mathrm{X}}m_{\mathrm{Y}}}$ $6_{\mathrm{Z}}'/\mathrm{m_{\mathrm{Z}}m_{\mathrm{X}}m_{\mathrm{Y}}'}$					