ES190 Final Project

Pentagonal Crystal System : Plausible Properties and Applications of 5 fold Rotational Symmetry

Billy Koech
Electrical Engineering SB
Harvard University
Cambridge, Massachussets
United States of America

***Abstract*— 5-fold rotation symmetry is exhibited in quasicrystals, but a 5-fold crystal system does not exist. The aim of this paper is to propose the possible structure and properties of point groups of a crystal system with 5-fold rotation. An assumption is made that 5-fold rotational symmetry is possible and derivations are done based on this assumption in order to show the 1st rank and 2nd rank tensor properties of the point groups that belong to this crystal systems. The last section is dedicated to discussing the possible applications of 5-fold rotational symmetry crystals based on the properties of quasicrystals.**

Keywords*— *pentagonal, quasicrystal, 5-fold, pyromagnetism, pyroelectricity, thermal expansion matrix

I. INTRODUCTION

According to the crystal restriction theorem crystals can only show 2-fold, 3-fold, 4-fold or 6-fold rotational symmetry[1],[2]. However, quasicrystals (discovered in the 1980s) have been found to naturally exhibit 5-fold[3] rotational symmetry although aperiodic[4]. This is the motivation behind this paper; we explore the question: what if 5-fold rotational symmetry was possible? This paper proposes that 5-fold rotational symmetry would give rise to a new crystal system: The pentagonal crystal system.

This paper is structured as follows: Using the nomenclature of the two closest crystal systems (Hexagonal and Tetragonal) the first section walks through the derivation of the point groups of such a crystal system and the corresponding the stereograms. It then transitions to derivations of metrices for the first and second ranks tensor properties (pyroelectricity, pyromagnetism and thermal expansion). The final section explores some possible applications for pentagonal crystals.

II. PENTAGONAL POINT GROUPS

A. *Point Group Derivation*

Assuming the possibility of 5-fold rotation, the pentagonal crystal would consist of the following point groups: 5, 5/m, 522, 5mm, 5/mmm. These 5 are chosen based on the pattern exhibited by two closest crystal groups – Tetragonal (4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}$2m, 4/mmm) and Hexagonal (6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}$m2, 6/mmm).

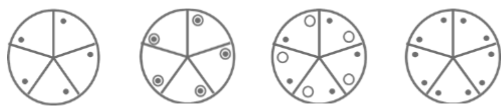
In comparison to hexagonal and tetragonal, the pentagonal group does not include inversion (such as $\bar{5}$) because such an operation would violate the symmetry as proven in the stereograms in Fig. 1. Furthermore, we propose the following notation for pentagonal which slightly differs from that of Hexagonal and Tetragonal:

- 1st notation is along the *c* axis
- 2nd notation is along or perpendicular to the *a* axis. The *a* axis must be aligned with the stereogram's rotation edge.
- 3rd notation is along or perpendicular to 28 degrees from the *b* axis

In the sections that follow, we focus on derivation of properties for just the first 4 point groups (5, 5/m, 522, 5mm)

B. *Stereograms*

Following the convention defined above, the following stereograms can be constructed for each point group:



5 5/m 522 5mm

Fig. 1. Stereograms for the pentagonal point groups

C. *Transformation matrices*

The transformation matrix for 5-fold rotation about the c axis is derived from the general formula for angular rotation about *c* where $\theta = 72°$:

$$R(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0.309 & 0.9511 & 0 \\ -0.9511 & 0.309 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Following the syntax and notation for the pentagonal point groups, the following transformation matrices are derived from multiplication of the individual symmetrical operations:

TABLE I. TRANFORMATION MATRICES

Point group	***Redundant element***	***Final matrix***
5	None	$\begin{pmatrix} 0.309 & 0.9511 & 0 \\ -0.9511 & 0.309 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
5/m	None	$\begin{pmatrix} 0.309 & 0.9511 & 0 \\ -0.9511 & 0.309 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
522	Last 2	$\begin{pmatrix} 0.309 & -0.9511 & 0 \\ -0.9511 & -0.309 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
5mm	Last m	$\begin{pmatrix} -0.309 & 0.9511 & 0 \\ 0.9511 & 0.309 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

III. FIRST RANK AND SECOND RANK TENSOR PROPERTIES

A. *Pyromagnetism, Pyrolectricity and Thermal Expansion Properties by Neumann's Principle*

The table below summarizes the results of applying Neuman's principle to derive the pyroelectric, pyromagnetic and thermal expansion matrices.

TABLE II. 1ST AND 2ND RANK TENSOR PROPERTIES

Point group	***Pyroelectric matrix***	***Pyromagnetic matrix***	***Thermal expansion matrix***
5	$\begin{pmatrix} 0 \\ 0 \\ p3 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ q3 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D33 \end{pmatrix}$
5/m	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ q3 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D33 \end{pmatrix}$
522	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D33 \end{pmatrix}$
5mm	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & D33 \end{pmatrix}$

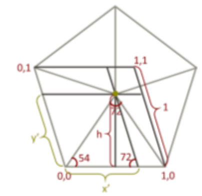
B. *Discussion*

Point group 5 allows for both pyroelectricity and pyromagnetism, both of which occur in the same crystallographic direction. 5/m allows for just pyromagnetism; it does not allow pyroelectricity. All the other point groups do not allow pyroelectricity or pyromagnetism.

All the point groups exhibit the same form for the thermal expansion matrix therefore they should also have similar strain matrices when subjected to a temperature change ΔT.

IV. BRAVAIS LATTICE AND STRUCTURE FACTOR

Based on observations of lattice diagrams, pentagonal vaguely resembles hexagonal. The Bravais lattice of a pentagonal system would likely be primitive and it would resemble the hexagonal primitive lattice except the cross section of the unit cell would not be a parallelogram. Consequently, the lattice would have two non-equivalent points. These nonequivalent points (calculated below) are (0,0,0) and at (0.7236,0.7236,0).



$$tan(54) = h/0.5$$
$$h = 0.6881$$
$$sin(72) = 0.6881/y'$$
$$y' = x' = 0.7236$$

a) Pentagonal primitive cell cross-section

b) Solution for 2nd nonequivalent point

Fig. 2. Derivation of the 2nd nonequivalent point for pentagonal primitive lattice

With the two nonequivalent points, the structure factor can be calculated as shown below:

$$F_{hkl} = \sum_{j=1}^{N} f^j \, e^{2\pi i\,(hx_j + ky_j + lz_j)}$$

$$F_{hkl} = f\,(e^{2\pi i\,0} + e^{2\pi i\,*1.4472\,(h+k)}) \approx f\,(1 + e^{2\pi i\,*1.5\,(h+k)})$$

$$F_{hkl} \approx \begin{cases} 0, & 1.5(h+k)\ is\ odd \\ 2, & 1.5(h+k\ )\ is\ even \end{cases}$$

V. POTENTIAL APPLICATIONS

Flexible magnets: 5 and 5/m have ferromagnetic properties, furthermore, the pentagon lattices can be arranged in such a way that the structure resembles that of polysiloxanes[5]. If this structure is possible then the crystal could potentially be magnetic and compliant.

Quasicrystals: Quasicrystals exhibit ordered but aperiodic 5-fold rotation. They also exhibit properties such as high thermal[6] and electrical resistance, low coefficient of friction[7] and non-stick properties that enables them to be applied in making non-stick frying pan coating[7], reinforcing steel[8] to make hard steel that's resistant to corrosion, and embedding in plastic to make hard low friction plastic gear. It is plausible that crystals of the pentagonal crystal system could also possess these properties and have these applications.

REFERENCES

[1] J. Bamberg, G. Cairns, and D. Kilminster, "The Crystallographic Restriction, Permutations, and Goldbach's Conjecture," *The American Mathematical Monthly*, vol. 110, no. 3, pp. 202–209, Mar. 2003.

[2] Z. Yue, "A Rigorous Proof on the Crystallographic Restriction Theorem to Establish Human Being," *Budapest International Research and Critics Institute (BIRCI-Journal) : Humanities and Social Sciences*, vol. 1, no. 4, pp. 25–28, Dec. 2018.

[3] C. Radin, "Symmetries of Quasicrystals," *Journal of Statistical Physics*, vol. 95, no. 5, pp. 827–833, Jun. 1999.

[4] I. Hargittai, "Dan Shechtman's Quasicrystal Discovery in Perspective," *Israel Journal of Chemistry*, vol. 51, no. 11–12, pp. 1144–1152, 2011.

[5] "Silicones." [Online]. Available: https://pslc.ws/macrog/silicone.htm. [Accessed: 05-Dec-2019].

[6] F. Schurack, J. Eckert, and L. Schultz, "Synthesis and mechanical properties of cast quasicrystal-reinforced Al-alloys," *Acta Materialia*, vol. 49, no. 8, pp. 1351–1361, May 2001.

[7] A. I. Goldman and M. Widom, "Quasicrystal Structure and Properties," *Annual Review of Physical Chemistry*, vol. 42, no. 1, pp. 685–729, 1991.

[8] V. V. Tcherdyntsev, S. D. Kaloshkin, E. V. Shelekhov, A. I. Salimon, S. Sartori, and G. Principi, "Quasicrystalline phase formation in the mechanically alloyed Al–Cu–Fe system," *Intermetallics*, vol. 13, no. 8, pp. 841–847, Aug. 2005.