Algebra of Close Packed Polytypes

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We all have stacked blocks since we were child !!

And we know is fairly easy !!!
So we do it all the time !!!
And so does nature !!!
Even at the atomic scale !!!
Polytypes deals with crystal made out of the stacking of identical two-dimensional periodic layers.

NdFeB
Polytypes

Sm2Co17
Close Packed Structure
Close Packed Structure
Close Packed Structure
Close Packed Structure
Close Packed Structure
Close Packed Structure

Same environment
Close Packed Structure

Different environments

A B C A B C

K K K K K K K K K
Close Packed Structure
Polytypes

For the purposes of this lecture two different crystals belong to the same polytypic family if they are constructed by the same two dimensional layers but with a different stacking arrangement.

![Diagram showing different stacking arrangements for polytypes](image)
Sir Walter Raleigh

Thomas Harriot

Johannes Kepler (1571-1630)
1611 - Christmas Card
Strena, Seu de Nive Sexalunga

Thomas Hales (M.I.T.) 1998

387 years after Kepler !!!
Nickel Cannon Balls
Polytypes

Politipo:

CBAB  BCBA

ABCB  BABC
Sequence Reversion
Equivalent Sequence

A B C B
B C B A
C B A B
B A B C

Reversed
HK notation

\[ H = 1 - \frac{\sum b_i}{N} \]
Hagg Notation

A + B → C
Hagg Notation

A

B

C
The Hagg notation is a less redundant notation that the ABC notation and therefore more compact. More importantly, it allow us to traduce the polytype problem to a mathematical problem that can be approached trough number theory, coding and information theory.
Hagg notation: Equivalence relations

Two Hagg codes are equivalent if …

1) … they can be brought into coincidence by a cyclic shift of the code. \( \hat{n} \)

2) … they can be brought into coincidence by a reversion of the code. \( \hat{P}I \)

3) … they can be brought into coincidence by the permutation of the two digits. \( \hat{P} \)
Hagg notation: Neutrality condition

\[
\#_s (|> N) \equiv \#_1 (|> N) - \#_0 (|> N) = 0 \mod 3
\]
Hagg notation: Neutrality condition

Any neutral $|>_{N}$ code can be obtained from a non-neutral code $|>_{N-1}$ of length N-1 if we add at the end a 1 or a 0. Two cases are possible:

$|>_{N} = |>_{N-1} \oplus 1 \quad \#_{s}(|>_{N-1}) = 2 \mod 3$

$|>_{N} = |>_{N-1} \oplus 0 \quad \#_{s}(|>_{N-1}) = 1 \mod 3$

There are $2^{N-1}$ possible codes of length N-1 of which $\Omega(N-1)$ will be neutral therefore will be $2^{N-1} - \Omega(N-1)$ codes from which we can construct a neutral code of length N.

$\Omega(N+1) = 2^{N} - \Omega(N)$

$\Omega(N+2) = 2^{N+1} - \Omega(N+1)$

$\Omega(N+3) = 2^{N+2} - \Omega(N+2)$

\[ \vdots \]

$\Omega(N+K) = (-1)^{K} \Omega(N) + \frac{1}{3} 2^{N} (2^{K} + (-1)^{K+1}).$
Hagg notation: Neutrality condition
Hagg notation: Zeitz operators

\[ \hat{S} = (S, | s >) \quad \hat{S} | b >_p = S | b >_p + | s >_p \]

Negation operator: \[ -\hat{P} = (\tilde{I}, | 2^p - 1 >) \]

Cyclic rotation: \[ \hat{p} = (\tilde{p}, | 0 >) \]

Reversion operation: \[ \hat{P} I = (\tilde{I}, | 0 >) \]

\[ \tilde{I} = \begin{pmatrix} 
0 & 0 & 0 & \ldots & 0 & 0 & 1 \\
0 & 0 & 0 & \ldots & 0 & 1 & 0 \\
0 & 0 & 0 & \ldots & 1 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 1 & \ldots & 0 & 0 & 0 \\
0 & 1 & 0 & \ldots & 0 & 0 & 0 \\
1 & 0 & 0 & \ldots & 0 & 0 & 0 
\end{pmatrix} \]

\[ \tilde{p} = \begin{pmatrix} 
0 & 0 & \ldots & 0 & 1 & 0 & \ldots & 0 \\
0 & 0 & \ldots & 0 & 0 & 1 & \ldots & 0 \\
0 & 0 & \ldots & 0 & 0 & 0 & \ldots & 1 \\
1 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
0 & 1 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & \ldots & 1 & 0 & 0 & \ldots & 0 
\end{pmatrix} \]
Hagg notation: Zeitz operators

Negation operator: $-\hat{P} = (\tilde{I}, |2^P - 1>)$

Unary shift operation: $\hat{1} = (\tilde{1}, |0>)$

Reversion operation: $\hat{P}I = (\tilde{I}, |0>)$

The action of $\diamondsuit\hat{\Box}_p$ over the set of all possible codes of length $P$ will classify each code into a family of orbits of codes, each family representing the same polytype.
$\mathcal{P}_p$: Hagg sequence group

Negation-rotation operator: $-\hat{p} = (\tilde{I}, |2^p - 1>)$

Rotation operation: $\hat{p} = (\tilde{p}, |0>)$

Reversion-rotation operation: $\hat{p}I = (\tilde{I}, |0>)$
\( \mathbb{P}_p \): Hagg sequence group

\[
\begin{align*}
\{-\hat{P}\} & \quad \text{Subgroup of order } 2 \\
\{\hat{P}I\} & \quad \text{Subgroup of order } 2 \\
\{\hat{p}\} & \quad \text{Subgroup of order } p \\
\{\hat{p}I\} & \quad \text{Does not form a subgroup but …} \\
\{\hat{p}I\} + \{\hat{p}\} & \equiv \{\hat{p}I\}^2 \quad \text{forms a subgroup of order } 2 \\
\{-\hat{p}\} & \quad \text{Does not form a subgroup but …} \\
\{-\hat{p}\} + \{\hat{p}\} & \equiv \{\pm\hat{p}\} \quad \text{forms a subgroup of order } \frac{P\gcd(P,p)}{2} \text{ if such division is even and } \frac{2P\gcd(P,p)}{2} \text{ otherwise}
\end{align*}
\]
Burnside lemma (Cauchy-Frobenius lemma): Let $G$ be a finite group of order $\#G$ permuting a finite set $K$ of elements, then

$$\Gamma(K) = \frac{1}{\#G} \sum_{g \in G} \#K_g$$

Where $\Gamma(K)$ is, under the action of $G$, the number of non-equivalent members of $K$. $K_g$ is the set of all elements of $K$ left fixed by $g$ and $\#K_g$ is the order of $K_g$. 
Following the Burnside lemma, the problem of counting the number of distinctive polytypes of length $P$ involves finding a formula for $\#_{\mathcal{K}_g}$, for all $g$ belonging to $\mathcal{T}_P$, where now $\mathcal{K}$ stands for all neutral codes of length $P$.

$$\Gamma(P) = \frac{1}{4P} \sum_{p=1}^{P} \left\{ \#_{\mathcal{K}_{\hat{p}}} + \#_{\mathcal{K}_{\hat{p}^{-1}}} + \#_{\mathcal{K}_{\hat{p}I}} + \#_{\mathcal{K}_{\hat{p}^{-1}I}} \right\} - \sum_{d_i} \Gamma(P / d_i)$$

$d_i$ : divisor of $P$
Counting polytypes

\( \#_{K_g} \) can be obtained from:

\[ \hat{S} \mid b \geq b > \text{mod} \ 2 + \]

Neutrality condition
Counting polytypes: Example

\[ \hat{3} | b >_{15} \equiv | b >_{15} \mod 2 \]

\[ | b >_{15} = | b_1 b_2 b_3 b_1 b_2 b_3 b_1 b_2 b_3 b_1 b_2 b_3 > \]

\[ 5(b_1 + b_2 + b_3) = 0 \mod 3 \quad \Omega(3) \]
Counting polytypes

When all independent characters \( \{f_i\} \) have the same multiplicity \( \#_m \), the neutrality condition will be

\[ \#_m \sum_i f_i = 0 \mod 3 \]

Two cases:

\[ \#_m = 3z \quad 2\#_f \]
\[ \#_m \neq 3z \quad \Omega(\#_f) \]
Counting polytypes

When you have more than one multiplicity of the independent characters \( \{ f_i \} \) the number of cases increases, for \( \vartriangle \bowtie_p \) the only other case that appears is:

\[
\#_{m_1} \sum_{i} b_i + \#_{m_2} \sum_{i} b_i = 0 \pmod{3}
\]

<table>
<thead>
<tr>
<th>( #_{m_1} \mod 3 )</th>
<th>( #_{m_2} \mod 3 )</th>
<th>No. of neutral codes</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>( 2^{#<em>{f_1} + #</em>{f_2}} )</td>
</tr>
<tr>
<td>0</td>
<td>( \neq 0 )</td>
<td>( 2^{#<em>{f_1} \Omega(#</em>{f_2})} )</td>
</tr>
<tr>
<td>( \neq 0 )</td>
<td>0</td>
<td>( 2^{#<em>{f_2} \Omega(#</em>{f_1})} )</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>( \Omega_2(#<em>{f_1}) \Omega_1(#</em>{f_2}) )</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>( +\Omega_1(#<em>{f_1}) \Omega_2(#</em>{f_2}) + \Omega(#<em>{f_1}) \Omega(#</em>{f_2}) )</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>( \Omega_2(#<em>{f_1}) \Omega_2(#</em>{f_2}) )</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>( +\Omega_1(#<em>{f_1}) \Omega_2(#</em>{f_2}) + \Omega(#<em>{f_1}) \Omega(#</em>{f_2}) )</td>
</tr>
</tbody>
</table>
Counting polytypes

\[ \Gamma(N) \]

\[ N \]

\[ 2.09715E6 \]

\[ 262144 \]

\[ 32768 \]

\[ 4096 \]

\[ 512 \]

\[ 64 \]

\[ 8 \]

\[ 1 \]

\[ 0 \]

\[ 5 \]

\[ 10 \]

\[ 15 \]

\[ 20 \]

\[ 25 \]

\[ 30 \]
Polytypes symmetry
Polytypes symmetry

Symmetry operations:
1) 3 rotation axis
2) 6 rotation axis
3) -1 inversion center
4) Mirror planes
Polytypes symmetry: $3_k$ axis

$\kappa \#_s (| r >) = 0 \mod 3$

Identity operator $3_1$
Polytypes symmetry: $6_k$ axis

$$k\#_s (\mid r >) = 0 \mod 3$$

$6_3$
Polytypes symmetry: $\bar{1}$ axis
Polytypes symmetry: mirror
Polytypes symmetry: $3_1 + \bar{1}$

\( \text{R}\bar{3}m \)
Polytypes symmetry: $6_3 + m$

There is an inversion center to !!
Polytypes symmetry: $3_1 + m$

Nothing new, the same as only a mirror !!!
Polytypes symmetry: $3_1 + 6_3$

Nothing new, the same as only the $6_3$ axis !!
Polytypes symmetry

Diagram showing the relationship between different polytypes and their symmetry groups.
Counting polytypes by symmetry

\[ \hat{S} \mid b \geq \mid b \rangle \mod 2 \]
\[ \hat{G} \mid b \geq \mid b \rangle \mod 2 \]

+ Neutrality condition
Polytypes symmetry

Grupo Espacial
- P3m1
- P3m1
- P6/mmc
- P6/m2
- P6/mc
- R3m
- R3m

Cantidad de códigos

N
Zhdanov Symbol

Run length encoding!!

110010 $\rightarrow$ 2211

110110110 $\rightarrow$ (21)$_3$

1010110110110 $\rightarrow$ (11)$_2$(21)$_3$
Information conveyed by the polytype

(21)_3
(21)_3(21)_3
(21)_3(21)_3(21)_3
(21)_3(21)_3(21)_3(21)_3

...
Information conveyed by the polytype

$(21)_3$
$(21)_311$
$(21)_31122$
$(21)_3112241$

...
Information conveyed by the polytype

The number of words in the Zhdanov symbol is a measure of the complexity of the polytype.
Information conveyed by the polytype

Alan Turing (1912-1954)
Kolmogorov complexity

\[ K(\text{polytype}) = |s^*| \]

The Kolmogorov complexity is the length of the shortest program capable of reproducing the entire system faithfully.
Information conveyed by the polytype

The input program is the same for all close packed polytypes.

The difference is the input data.

The Zhdanov symbol !!
Information conveyed by the polytype

20 layers

50 layers

100 layers