Theory of Groups and *coset decomposition*

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Outlook

- Introduction
- Brief historical account
- A non-rigorous mathematical *exposé*
- A paraphrase of Flack (1987) : Twins and coset decomposition of point groups
- Conclusion
- An exercise using Jana2006

Introduction

(Pseudo-)merohedral twins :

- several descriptions may be used to describe a particular twin
- several distinct twins may be expressed simultaneously

Group theory and coset description of point group allow to :

- check all possibilities of twins using the metrical information on the lattice
- check the orientation of the structure / lattice

Brief historical account

- Joseph-Louis Lagrange (1771)
  Algebraic equations
  Some ideas about groups

- Evariste Galois (1830) → 1850
  Algebraic equations - group theory
  Coset decomposition

- Developpements of group theory (Felix Klein – 1872 ...)

- Sohnke (1867) → Schönflies-Fedorov (~ 1890)
  Space groups

- George Friedel (1904)
  Twins

- 1970's and 80's : use of coset decomposition / twins

Mathematical introduction

Roots of a polynom

Example : Z a complex number ; $Z^n = 1$

$$Z = e^{i2\pi k/n}, k = 0,1...(n-1)$$

Links between geometry and algebra

Group theory

• **Definition of a group** :

An ensemble with a composition law (closure relation) and :

- **associativity**
- **existence of a neutral element**
- **existence of an inverse**

Not necessary commutative (if commutative, the group is called abelian)

May be finite or not

• **Order of the group:** **its cardinal** ***card*(G)**

• **Multiplication table** **(finite groups)**

• **Abstract group**

• **Subgroup / supergroup**

Crystallographic point groups :

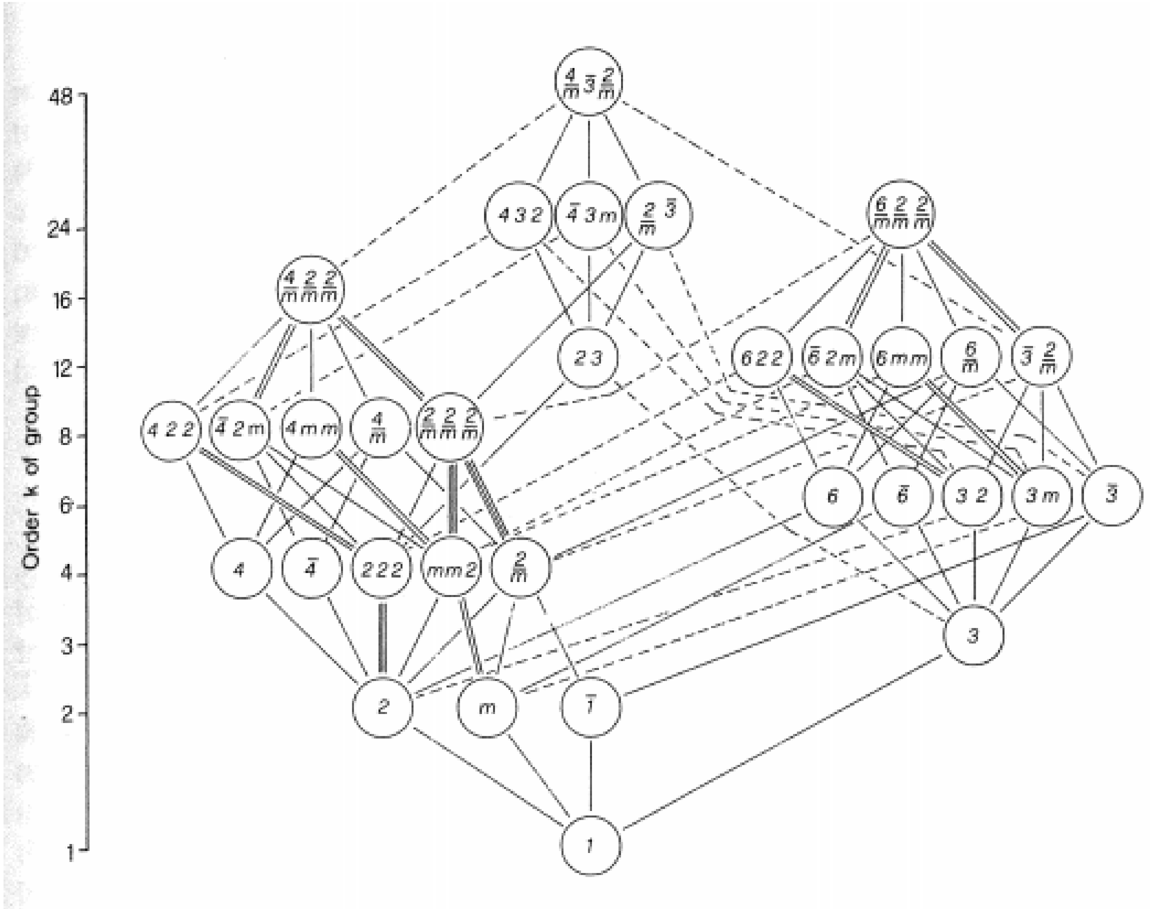
Table 1.E.2 The 18 abstract groups corresponding to the 32 crystallographic point groups

Point group	Order of the group	Characteristic relations
1	1	$g = e$
$\bar{1}$, 2, *m*	2	$g^2 = e$
3	3	$g^3 = e$
4, $\bar{4}$	4	$g^4 = e$
2/*m*, *mm*2, 222	4	$g_1^2 = g_2^2 = (g_1g_2)^2 = e$
6, $\bar{6}$, $\bar{3}$	6	$g^6 = e$
32, 3*m*	6	$g_1^3 = g_2^2 = (g_1g_2)^2 = e$
mmm	8	$g_1^2 = g_2^2 = g_3^2 = (g_1g_2)^2 = (g_1g_3)^2 = (g_2g_3)^2 = e$
4/*m*	8	$g_1^4 = g_2^2 = g_1g_2g_1^3g_2 = e$
4*mm*, 422, $\bar{4}2m$	8	$g_1^4 = g_2^2 = (g_1g_2)^2 = e$
6/*m*	12	$g_1^6 = g_2^2 = g_1g_2g_1^5g_2 = e$
$\bar{3}m$, $\bar{6}2m$, 6*mm*, 622	12	$g_1^6 = g_2^2 = (g_1g_2)^2 = e$
23	12	$g_1^3 = g_2^2 = (g_1g_2)^3 = e$
4/*mmm*	16	$g_1^2 = g_2^2 = g_3^2 = (g_1g_2)^2 = (g_1g_3)^2 = (g_2g_3)^4 = e$
432, $\bar{4}3m$	24	$g_1^4 = g_2^2 = (g_1g_2)^3 = e$
$m\bar{3}$	24	$g_1^3 = g_2^2 = (g_1^2g_2g_1g_2)^2 = e$
6/*mmm*	24	$g_1^2 = g_2^2 = g_3^2 = (g_1g_2)^2 = (g_1g_3)^2 = (g_2g_3)^6 = e$
$m\bar{3}m$	48	$g_1^4 = g_2^6 = (g_1g_2)^2 = e$

From : Giacovazzo, C.; Monaco, H. L.; Artioli, G.; Viterbo, D.; Ferraris, G.; Giacovazzo, C. *Fundamentals of Crystallography*; Oxford University Press, Oxford, 2002

Group theory

Group, subgroup, supergroup relationships for crystallographic point groups :



From International Tables of Crystallography

Group theory: Cosets and coset decomposition

Definition : H = {*h1, h2*…} subgroup of G. Let *g* be a an element of G **contained or not** in H.
g.H = {*g.h1, g.h2, …*} is a **left coset**
H.g = {*h1.g, h2.g, …*} is a right coset

Trivial cosets : H himself; if H = {*e*} … ; if H = G…

Definition : an **equivalence relation** is a binary relation, which is **reflexive**, **symmetric**, and **transitive**. Such an equivalence relation allow to define **equivalence classes** in an ensemble and to define a **partition** (of this ensemble).

Theorem : Let *a* and *b* be elements of G. The relation *a ~ b*, if there exist an element h of H such that *a=b.h*, is an **equivalence relation**. In other words, the **left cosets of H in G form a partition of G.** This is called a left **coset decomposition** of G in H.

Left *cosets* = *classes (latérales)* à gauche

Group theory: Coset decomposition

H subgroup of G. Left coset decomposition of G in H :

$$G = e.H \cup g_1.H \cup \ldots$$

Example 1 : $2/m = (1,2,\bar{1},m) = 1.(1,2) \cup \mathrm{m}.(1,2)$

$$2/m = 1.(1,2) \cup \bar{1}.(1,2)$$

A coset decomposition is unique, but the system of representatives is not.

Example 2 : (left) coset decomposition of relative integers in even (relative) integers

→ coset decomposition of an infinite group into two infinite groups

Lagrange's theorem : H subgroup of G (finite). The order of H divides that of G.
P = card (G)/card(H) is called the **index of H** relative to G and is noted **[G:H].** It corresponds to the number of left (right) cosets of H in G

Proof : use cosets…

[G:H] being the number of cosets, this allows to generalize the concept of index to infinite groups. See previous example2.

Definition : H **proper (=invariant) subgroup** of G : for each g of G, $g^{-1}.H.g=H$

This is equivalent to say that $g.H = H.g$ for each g of G, i.e., left and right cosets are equal.

Group theory : factor group

H is a normal subgroup of G

G/H is an ensemble formed by the cosets of H in G

We define a composition law o :
{g.H}o{f.H} = g.H.f.H where g and f are two elements of G

o is an internal composition law :
g.H.*f*.H = *g*.H.H.*f* = *g*.H.*f* = *g*.*f*.H is also a coset of H in G (*g*.*f* is an element of G)

o is associative, admits a neutral element (H), and an inverse for each element (i.e., each coset) → G/H is a group, called factor or quotient group

Example 1 : G = 4 = {1, 4, 2, 4^3}   H = {1, 2} G/H = {{1,2}, {4, 4^3}}

Example 2 : relative integers, E and O   G/H = {E, O}

G → G/H is an example of homorphism ("many to a few")

Twins and coset decomposition – Flack (1987)

Flack, H. D. The Derivation of Twin Laws for (Pseudo-)Merohedry by Coset Decomposition. Acta Crystallographica Section A 1987, 43 (4), 564–568.
https://doi.org/10.1107/S0108767387099008

Central idea : for (pseudo-)merohedry : to perform a decomposition of the point group of the lattice into the (left) cosets of the point group of the crystal

This will allow to :
- check all possibilities of twin laws using the metrical information on the lattice
- check the orientation of the structure / lattice

In pseudo-merohedry, the metrically higher symmetry of the lattice is never exact and exists only within the experimental error.

Twins and coset decomposition – Flack (1987)

- **a coset decomposition is unique, but this is not necessarily the case for the representative of this coset (g_1.H = g_2.H with g_1 and g_2 different elements of G)**

- **same arbitrariness for the definition of twin laws**

The author proposes two algorithms to :

- follow some conventions in the description or twin laws (use twin axes rather than planes if this is possible)

- or to have a description of twins strongly bound to a centre of symmetry (nevertheless using twofold axis wherever possible)

Seven "Laue" point groups :

$$\bar{1},\ 2/m,\ mmm,\ 4/mmm,\ \bar{3}2m,\ 6/mmm,\ m\bar{3}m$$

Twins and coset decomposition – An example

Crystal : point group 2/m but lattice metrical information "almost" orthorhombic

Card (2/m) = 4 Card (mmm) = 8 [mmm:2/m] = 2
2 cosets

$$2/m = (1, 2_{[010]}, \bar{1}, \bar{2}_{[010]})$$

$$mmm = 1.2/m \bigcup \bar{2}_{[001]}.2/m$$

Conclusions

• for the case of (pseudo-)merohedry : the interest to have such an algorithm directly integrated into programs to analyze integrated twinned data

• the interest of coset decomposition of space groups in cristallography ?
- to analyse some phase transitions
- also for twin law analysis

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