



HAL
open science

Morphology of crystals developed in liquid and in solid media: Symmetry analysis -Group theory

Abdelkrim Redjaïmia, Anna Nominé Nominé, Hiba Kabbara, Jaâfar Ghanbaja, Thierry Belmonte

► **To cite this version:**

Abdelkrim Redjaïmia, Anna Nominé Nominé, Hiba Kabbara, Jaâfar Ghanbaja, Thierry Belmonte. Morphology of crystals developed in liquid and in solid media: Symmetry analysis -Group theory. International Conference of Mechanics and Materials (ICMM'2023), Université Ferhat Abbas - Sétif, Algérie, Nov 2023, Sétif, Algeria. hal-04296944

HAL Id: hal-04296944

<https://hal.univ-lorraine.fr/hal-04296944>

Submitted on 21 Nov 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Morphology of crystals developed in liquid and in solid media: Symmetry analysis – Group theory

ABDELKRIM REDJAÏMIA*

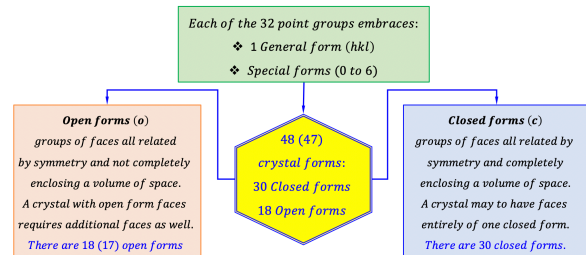
ANYA NOMINE, HIBA KABBARA, JAÂFAR GHANBAJA, THIERRY BELMONTE

Institut Jean Lamour, Université de Lorraine, UMR CNRS 7198, Nancy, F-54042, France

* Abdelkrim.redjaimia@univ-Lorraine.fr

ABSTRACT

This study points out how symmetry analysis, based on group theory, can be exploited to explain the morphology, the variant number, the variant directions, the habitus (habit plane) of crystal developing in different media (gas, liquid and solid). The elements necessary for symmetry analysis will be briefly presented. A practical use of the crystal symmetry will be presented and illustrated with two examples derived from transmission electron microscopy study: development of nanosheets of lead oxide and bismuth carbonate in a liquid media and precipitation of τ and χ intermetallic phases in a metallic matrix, the ferrite in ($\delta + \gamma$) duplex stainless steel.



Map. 1: The 32 point-groups embrace Crystal forms spread in: 143 (32 general, 111 special) shapes and 48 (18 open and 30 closed) forms.

KEY WORDS:

Crystal Symmetry; Shape; Point group; γ -PbO₂; (BiO)₂(OC)₃; χ – phase; τ – Phase; δ – matrix

I. INTRODUCTION

It is well established, through group theory, that the morphology of phases, taking place in any medium (solid, liquid or gas) is of great importance in materials science. The crystal form, the variant number and the habitus can be understood in terms of group theory [1, 2]. It is well known that the combination of the rotation symmetry axes (direct and roto-inverses) and the mirror leads to 32 point-groups. To each point group is associated 1 general (*hkl*) form and 0 to 6 special forms (Tab. 1&2). This combination allows to have 48 (47) forms. Among these forms, 30 are closed and 18 (17) are open (Map. 1). Taking into account the 7 crystal systems (Tab. 1), there are finally 143 forms among which 32 are general, 111 special, 18 (17) open and 30 closed (Tab. 2).

This symmetry concept has been successfully applied to determine the number of variants and to characterize the morphology of precipitates in different alloy systems, and is widely investigated [1, 2].

Crystal systems ⇒		Triclinic		Monoclinic		
Crystal forms (2 / 5)	# Faces	Point groups		Point groups		
		1	$\bar{1}$	2	<i>m</i>	2/ <i>m</i>
1. Pedion	1	<i>hkl</i>		010, 010	<i>h0l</i>	
2. Pinacoid	2		<i>hkl</i>	<i>h0l</i>	010	010, <i>h0l</i>
3. Sphenoid	2			<i>hkl</i>		
4. Dome	2				<i>hkl</i>	
5. Rhombic Prism	4					<i>hkl</i>
Class ⇒		Pedial	Pinacoidal	Sphenoidal	Domatic	Prismatic

Tab. 1: Crystal forms (general and special) versus the point groups (1, $\bar{1}$) and (2, *m*, 2/*m*) for the Triclinic and Monoclinic systems, respectively. One can notice that equivalent tables for the other crystal systems (orthorhombic, tetragonal, trigonal, hexagonal and cubic) can be derived without ambiguity.

Tab. 2: Occurrence (*f*) of crystal forms (closed, open, general and special) versus point groups (crystal systems).

The morphology of the crystal depends of the media in which it takes place:

@ In fluids (water, liquid nitrogen, *etc.*), considered as isotropic media, the morphology and the variant number of the developed crystal are dictated by the symmetry element of its point group.

@ Unlike the previous case, the shape of the crystal developing in solid media (metallic matrixes) is dictated by the point group whose symmetry elements are common to the point group of the matrix and of that of the precipitate.

Both the morphology and the variant number of the precipitate, which adopt orientation relationships (OR) with the matrix, are determined by the point group H_h ($H_h = G_m^M \cap G_p^P$), whose elements are common to G_m^M and G_p^P , the point groups of the matrix (M) and of the precipitate (P), respectively [1, 2].

This approach, based on the shared symmetry elements of the two point-groups can be applied to explain the habitus, the shape and especially the variant number n developed by the precipitate in the matrix. The latter is the ratio: $n = m/h$, where m and h are the order of the point group G_m^M and H_h , respectively [2].

II. RESULTS

A. SYMMETRY ANALYSIS AND MORPHOLOGY OF CRYSTAL DEVELOPED IN LIQUID (ISOTROPIC) MEDIUM

On the basis of the electron diffraction analysis, the $\gamma - PbO_2$, lead dioxide [3] and $Bi_2O_2CO_3$, bismuth sub-carbonate nanosheets [4], crystallize in the hexagonal and tetragonal systems, respectively. They belong to the $P6/mmm$ and $I4/mmm$ space groups, with $6/mmm$ and $4/mmm$ point groups (PG), respectively. These nanosheets develop hexagonal-prismatic and pinacoid shapes, respectively [Fig.1]. Both are special open forms [Tab.1].

B. SYMMETRY ANALYSIS AND MORPHOLOGY OF CRYSTAL DEVELOPED IN SOLID MEDIUM, A METALLIC MATRIX ($\delta - FERRITE$)

On the basis of the electron diffraction analysis, the $\tau - phase$ [5] and $\chi - phase$ [6], crystallize in the orthorhombic and cubic systems, respectively. They belong to the $Fmmm$ and $I\bar{4}3m$ space groups, with mmm and $\bar{4}3m$ point groups, respectively. Based on the orientation relationships, Bain and Cube-Cube between the ferritic matrix and τ and χ [5, 6], these phases develop rhombic prism and rhombic dodecahedron, respectively [Fig. 2]. The former is open form while the latter is closed form [Tab.1].

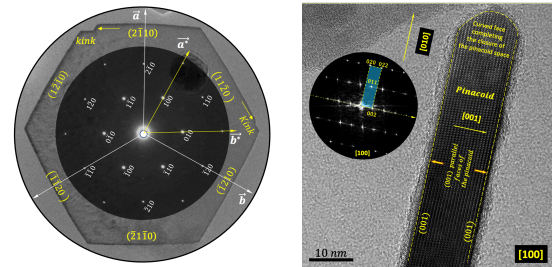


Fig. 1. Bright field TEM images of: **a)** $\gamma - PbO_2$, with superimposed its corresponding electron diffraction: Hexagonal prismatic (special open, $f = 10$) shape. **b)** HREM-TEM image of $Bi_2O_2CO_3$, Pinacoid (special open, $f = 20$) shape; where f is the occurrence of the shape.

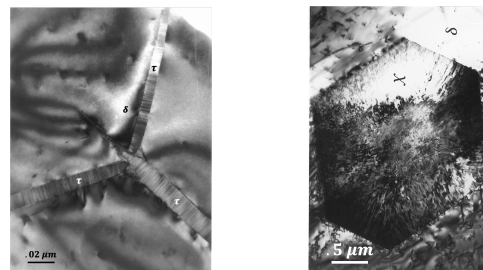


Fig. 2. BF-TEM Images of **a)** 3 lenticular variants of $\tau - phase$: Rhombic prism (special open; $f = 4$) shape. **b)** $\chi - phase$ particle Rhombic dodecahedron (special closed, $f = 5$) shape.

III. CONCLUSION

Hexagonal prism and pinacoid developed in the liquid (isotropic) medium and rhombic prism and rhombic dodecahedron, developed in solid medium (ferritic matrix), correspond to an absolute extremum, indicating that the growth of these phases is energetically favourable, *i.e.*, stables.

REFERENCES

- [1] M.J. Buerger, Elementary Crystall., Massachusetts Institute of Technology Press, Cambridge (1978).
- [2] J.W. Cahn, G. Kalonji, Proc. of the Inter. Conf. on Solid-Solid Phase Transformations, ed. by H. I. Aaronson, R. F. Sekerka, D. E. Laughlin & C.M. Waymann, pp. 3–14. Warrendale, TMS-AIME, (1982)
- [3] H. Kabbara *et al.*, Crystal structure, morphology and formation mechanism of a novel polymorph of lead dioxide, $\gamma - PbO_2$, J. Appl. Cryst. 52, 304–311 (2019).
- [4] A. Nomine *et al.*, Structural characteristics of $Bi_2O_2CO_3$ nanosheets synthesized by nano-pulsed discharges in water, Submitted to J. Appl. Cryst (2023).
- [5] A. Redjaïmia, *et al.*, Identification and characterization of a novel intermetallic compound in Fe-22Cr5Ni3Mo0.03C wt.% duplex ($\delta + \gamma$) stainless steel. Philos. Mag. A, 67, 1277–1286 (1993).
- [6] A. Redjaïmia *et al.*, Morphology, crystallography and defects of the intermetallic χ -phase precipitated in a duplex ($\delta + \gamma$) stainless steel, J. Mater. Sci. 39, 2371–2386, (2004).