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

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## 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  $\tau$  and  $\chi$  intermetallic phases in a metallic matrix, the ferrite in ( $\delta + \gamma$ ) duplex stainless steel.*

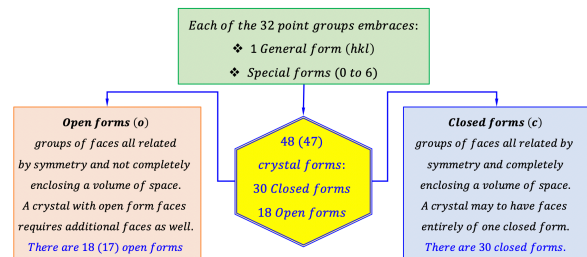
## KEY WORDS:

Crystal Symmetry; Shape; Point group;  $\gamma$ -PbO<sub>2</sub>; (BiO)<sub>2</sub>(OC)<sub>3</sub>;  $\chi$  – phase;  $\tau$  – Phase;  $\delta$  – 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].



**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.

Crystal systems ⇒		Triclinic			Monoclinic	
Crystal forms (2 / 5)	# Faces	Point groups			Point groups	
		1	$\bar{1}$	2	$m$	$2/m$
1. Pedion	1	$hkl$		010, 010	$h0l$	
2. Pinacoid	2		$hkl$	$h0l$	010	010, $h0l$
3. Sphenoid	2			$hkl$		
4. Dome	2				$hkl$	
5. Rhombic Prism	4					$hkl$
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].

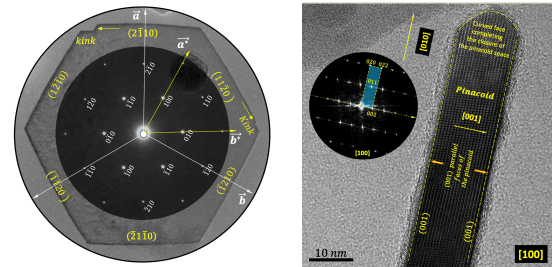
## II. RESULTS

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

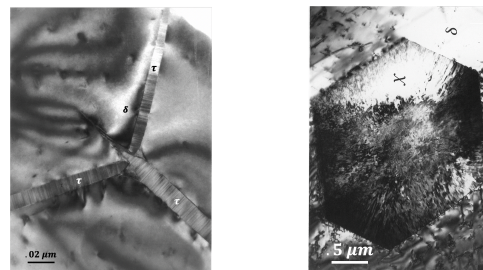
On the basis of the electron diffraction analysis, the  $\gamma - PbO_2$ , lead dioxide [3] and  $Bi_2O_2CO_3$ , bismuth sub-carbonate nanosheets [4], crystallize in the hexagonal and tetragonal systems, respectively. They belong to the  $P6/mmm$  and  $I4/mmm$  space groups, with  $6/mmm$  and  $4/mmm$  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  $\tau$  and  $\chi$  [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.

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