# Supplementary material 3:

# The use of groupoid composition table to define crystallographic packets of martensitic variants in Kurdjumov-Sachs orientation relationship.

Kurdjumov-Sachs (KS) is the most often reported orientations relationship (OR) in steels and iron alloys. For a long time, metallurgists tried to classify some peculiar arrangements or configurations of KS variants. Gourgues *et al*. (2000) and Lambert-Perlade *et al*. (2004) introduced the notion of morphologic and crystallographic packets, and few later Morito *et al.* (2003, 2006) defined blocks and packets. One must be very careful with those terms, for example the "crystallographic packets" defined by Gourgues *et al.* (2000) are assembly of variants linked by low misorientations; they constitute therefore what is sometimes called "Bain zones", whereas "packets" are now often used to designate other crystallographic packets, i.e. the sets of 6 variants that share a common $(111)_\gamma = (110)_\alpha$ plane which is also close to the habit plane for low carbon steels (Morito *et al*., 2003). The blocks are pairs of variants interrelated by a $60°/[110]_\alpha$ rotation in a packet and forming parallel laths with similar contrast in optical microscopy (Morito *et al*., 2006). We have represented in the Fig. S3_1 the 24 KS variants corresponding to the Table S3_2 and Table S3_1 such that the $\{111\}_\gamma$ faces of the γ parent phase are in white and the $\{110\}_\alpha$ planes in green. Three special configurations, close-packed plane (CPD), close-packed direction (CPP) and Bain, are marked in yellow and detailed in the following.

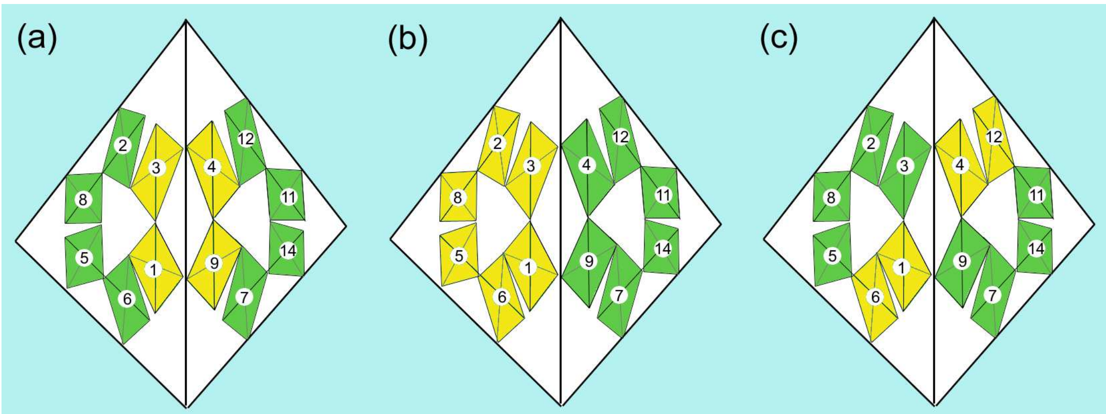


*Fig. S3_1. Three important crystallographic packets of KS variants represented in 3D and marked in yellow: (a) a CPD packet, (b) a CPP packet and (d) a Bain packet.*

The aim of the Supplementary section is to give a rigorous definition of Bain, CPP and CDD packets on the base of groupoid approach.

# 1 The groupoid of KS variants

Before defining the packets, the groupoid of KS variants must be established. The reader not familiar with groups or their extension to groupoids should not be afraid by the vocabulary and understand the terms “groups” or “groupoids” as “sets” or “packets”. A groupoid can be simply explained by geometry; it is just a set of objects (here the variants) linked by arrows (the misorientations). The sets of equivalent arrows (i.e. arrows between pairs of variants equivalently misoriented) are called operators. The groupoid composition is a very intuitive law: an arrow from a variant *i* to a variant *j* can be composed with an arrow from variant *j* to variant *k* and the result is the arrow from the variant *i* to the variant *k*, which can be written $[\alpha_i \rightarrow \alpha_j]\ [\alpha_j \rightarrow \alpha_k] = [\alpha_i \rightarrow \alpha_k]$. The arrows from variant *i* to variant *j* can be inverted $[\alpha_i \rightarrow \alpha_j]^{-1} = [\alpha_j \rightarrow \alpha_i]$, and each variant *i* has is own neutral element which is the circular arrow $[\alpha_i \rightarrow \alpha_i]$. Groupoids are more generalised than group and are the best mathematical tool to describe a geometrical figure with its own global symmetry but locally composed of objects that have their own symmetry. Those notions can be translated into algebraic terms by decomposing of groups into cosets, double-cosets. See (Cayron, 2006) for more details.

Let $\mathbf{G}^\gamma$ and $\mathbf{G}^\alpha$, the groups of symmetries of the $\gamma$ and $\alpha$ phases, and T the transformation matrix of the parent $\gamma$ crystal to a $\alpha$ daughter crystal, which encodes the OR. The symmetries common to both the parent and daughter crystals forms a subgroup of $\mathbf{G}^\gamma$ given by $\mathbf{H}^\gamma = \mathbf{G}^\gamma \cap \mathrm{T}\, \mathbf{G}^\alpha\, \mathrm{T}^{-1}$. The variants are expressed by cosets of type $\alpha_i = g_i^\gamma\, \mathbf{H}^\gamma$ with $g_i^\gamma \in \mathbf{G}^\gamma$ and encoded by set of matrices. The orientation of variant *i* is given by the set of equivalent matrices $\alpha_i$T. The number of variants results from Lagrange's formula $\mathrm{N}^\alpha = |\mathbf{G}^\gamma|/|\mathbf{H}^\gamma|$. With the KS OR there is only two common symmetries, the identity and inversion symmetry, such that the order of $\mathbf{H}^\gamma$ is two and the number of variants is 48/2 = 24. The distinct disorientations between the variants, i.e. the operators, are expressed by double cosets, also encoded by set of matrices. Their number is given by the Burnside formula. There are 23 operators between the 24 KS variants, counting the operator identity and distinguishing the polar operators. A polar operator is expressed by a set of equivalent rotations that is distinct of the set of inverses rotations. These 23 operators were calculated with a dedicated computer program called GenOVa (Cayron, 2007b) and are given in Table S3_2. The set of variants and operators form the groupoid of orientational variants (Cayron, 2006). The whole information of this structure is encoded in the groupoid composition table is presented in Table S3_1. It can be read as follow. The vertical label is composed of operators $\mathrm{O}_m$ with the variants $\alpha_i$ such that $[\alpha_1 \rightarrow \alpha_i]$

belongs to the $O_m$. The horizontal label is composed of operators $O_n$ with the variants $\alpha_j$ such that the arrow $[\alpha_1 \rightarrow \alpha_j]$ belongs to $O_n$. The composition of operators is obtained, without matrix calculation, directly by the groupoid law: $(O_m)^{-1}O_n$ are all the operators that contain the arrows $[\alpha_i \rightarrow \alpha_1]$ $[\alpha_1 \rightarrow \alpha_j]$ = $[\alpha_i \rightarrow \alpha_j]$. The product of operators is generally multivalued -see for example the groupoid composition table of NW variants (Cayron *et al.* 2006)-, but with KS OR the product is simply monovalued as a classical mathematical application is. For example $O_9^{-1}O_2 = [\alpha_{11} \rightarrow \alpha_1]$ $[\alpha_1 \rightarrow \alpha_3] = [\alpha_{11} \rightarrow \alpha_3] \in$ and = $O_{13}$ (see Table S3_2).

| | | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 5 | 3 | 4 | 2 | 6 | 16 | 8 | 9 | 11 | 10 | 17 | 18 | 15 | 14 | 7 | 12 | 13 | 19 | 24 | 21 | 22 | 23 | 20 |
| 0 | 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
| 1 | 5 | 4 | 0 | 7 | 10 | 1 | 2 | 3 | 5 | 13 | 18 | 6 | 8 | 9 | 11 | 22 | 17 | 23 | 20 | 12 | 14 | 15 | 16 | 19 | 21 |
| 2 | 3 | 2 | 7 | 0 | 8 | 5 | 4 | 13 | 1 | 3 | 14 | 11 | 10 | 22 | 6 | 9 | 16 | 15 | 21 | 19 | 18 | 23 | 17 | 12 | 20 |
| 3 | 4 | 3 | 9 | 8 | 0 | 15 | 16 | 17 | 14 | 2 | 1 | 12 | 22 | 10 | 21 | 7 | 4 | 5 | 6 | 20 | 23 | 18 | 13 | 11 | 19 |
| 4 | 2 | 1 | 4 | 5 | 6 | 0 | 7 | 10 | 2 | 11 | 12 | 3 | 13 | 18 | 8 | 19 | 20 | 21 | 15 | 9 | 22 | 17 | 23 | 14 | 16 |
| 5 | 6 | 5 | 2 | 1 | 11 | 7 | 0 | 8 | 4 | 6 | 19 | 13 | 3 | 14 | 10 | 12 | 21 | 20 | 23 | 22 | 9 | 16 | 15 | 18 | 17 |
| 6 | 16 | 15 | 3 | 14 | 12 | 9 | 8 | 0 | 16 | 21 | 20 | 17 | 2 | 1 | 22 | 11 | 6 | 19 | 18 | 10 | 7 | 4 | 5 | 23 | 13 |
| 7 | 8 | 7 | 5 | 4 | 13 | 2 | 1 | 11 | 0 | 10 | 22 | 8 | 6 | 19 | 3 | 18 | 23 | 17 | 16 | 14 | 12 | 21 | 20 | 9 | 15 |
| 8 | 9 | 8 | 14 | 3 | 2 | 16 | 15 | 21 | 9 | 0 | 7 | 22 | 12 | 11 | 17 | 1 | 5 | 4 | 13 | 23 | 20 | 19 | 6 | 10 | 18 |
| 9 | 11 | 10 | 18 | 13 | 4 | 17 | 23 | 20 | 22 | 7 | 0 | 9 | 19 | 6 | 16 | 5 | 1 | 2 | 3 | 15 | 21 | 12 | 11 | 8 | 14 |
| 10 | 10 | 9 | 15 | 16 | 17 | 3 | 14 | 12 | 8 | 22 | 10 | 0 | 21 | 20 | 2 | 23 | 18 | 13 | 4 | 1 | 11 | 6 | 19 | 7 | 5 |
| 11 | 17 | 16 | 8 | 9 | 22 | 14 | 3 | 2 | 15 | 17 | 23 | 21 | 0 | 7 | 12 | 10 | 13 | 18 | 19 | 11 | 1 | 5 | 4 | 20 | 6 |
| 12 | 18 | 17 | 10 | 22 | 9 | 18 | 13 | 4 | 23 | 16 | 15 | 20 | 7 | 0 | 19 | 8 | 3 | 14 | 12 | 6 | 5 | 1 | 2 | 21 | 11 |
| 13 | 15 | 14 | 16 | 15 | 21 | 8 | 9 | 22 | 3 | 12 | 11 | 2 | 17 | 23 | 0 | 20 | 19 | 6 | 5 | 7 | 10 | 13 | 18 | 1 | 4 |
| 14 | 14 | 13 | 22 | 10 | 7 | 23 | 17 | 16 | 18 | 4 | 5 | 19 | 9 | 8 | 20 | 0 | 2 | 1 | 11 | 21 | 15 | 14 | 3 | 6 | 12 |
| 15 | 7 | 6 | 12 | 11 | 1 | 20 | 21 | 15 | 19 | 5 | 4 | 18 | 14 | 3 | 23 | 2 | 0 | 7 | 10 | 17 | 16 | 9 | 8 | 13 | 22 |
| 16 | 12 | 11 | 19 | 6 | 5 | 21 | 20 | 23 | 12 | 1 | 2 | 14 | 18 | 13 | 15 | 4 | 7 | 0 | 8 | 16 | 17 | 22 | 10 | 3 | 9 |
| 17 | 13 | 12 | 20 | 21 | 15 | 6 | 19 | 18 | 11 | 14 | 3 | 1 | 23 | 17 | 5 | 16 | 9 | 8 | 0 | 4 | 13 | 10 | 22 | 2 | 7 |
| 18 | 19 | 18 | 17 | 23 | 20 | 10 | 22 | 9 | 13 | 19 | 6 | 4 | 16 | 15 | 7 | 21 | 12 | 11 | 1 | 0 | 8 | 3 | 14 | 5 | 2 |
| 19 | 24 | 23 | 13 | 18 | 19 | 22 | 10 | 7 | 17 | 20 | 21 | 16 | 4 | 5 | 9 | 6 | 11 | 12 | 14 | 8 | 0 | 2 | 1 | 15 | 3 |
| 20 | 21 | 20 | 6 | 19 | 18 | 12 | 11 | 1 | 21 | 23 | 17 | 15 | 5 | 4 | 14 | 13 | 10 | 22 | 9 | 3 | 2 | 0 | 7 | 16 | 8 |
| 21 | 22 | 21 | 11 | 12 | 14 | 19 | 6 | 5 | 20 | 15 | 16 | 23 | 1 | 2 | 18 | 3 | 8 | 9 | 22 | 13 | 4 | 7 | 0 | 17 | 10 |
| 22 | 23 | 22 | 23 | 17 | 16 | 13 | 18 | 19 | 10 | 9 | 8 | 7 | 20 | 21 | 4 | 15 | 14 | 3 | 2 | 5 | 6 | 11 | 12 | 0 | 1 |
| 23 | 20 | 19 | 21 | 20 | 23 | 11 | 12 | 14 | 6 | 18 | 13 | 5 | 15 | 16 | 1 | 17 | 22 | 10 | 7 | 2 | 3 | 8 | 9 | 4 | 0 |

*Table S3_1. KS groupoid table. The horizontal label (grey background) are operators $O_n$ (in black) with the variants $\alpha_j$ (in blue, below) such that the arrow $[\alpha_1 \rightarrow \alpha_j]$ belongs to $O_n$. The vertical label (grey background) are the operators $O_m$ with the variants $\alpha_i$ such that $[\alpha_1 \rightarrow \alpha_i]$ belongs to the $O_m$. The composition of operators is the operator in box (m,n) given by $(O_m)^{-1}O_n = \{O_p$ , $[\alpha_i \rightarrow \alpha_1]$ $[\alpha_1 \rightarrow \alpha_j] = [\alpha_i \rightarrow \alpha_j] \ni O_p$ }. Here the product is monovalued, for example $O_9^{-1}O_2 = [\alpha_{11} \rightarrow \alpha_1]$ $[\alpha_1 \rightarrow \alpha_3] = [\alpha_{11} \rightarrow \alpha_3] \in O_{13}$, and the KS groupoid can also be represented by a group.*

| | | |
|---|---|---|
| Op. 0 | Id. | [1, 1], [2, 2], [3, 3], [4, 4], [5, 5], [6, 6], [7, 7], [8, 8], [9, 9], [10, 10], [11, 11], [12, 12], [13, 13], [14, 14], [15, 15], [16, 16], [17, 17], [18, 18], [19, 19], [20, 20], [21, 21], [22, 22], [23, 23], [24, 24] |
| Op. 1 | 60.0° / [1 0 1] | [1, 5], [2, 1], [3, 8], [4, 11], [5, 2], [6, 3], [7, 4], [8, 6], [9, 14], [10, 19], [11, 7], [12, 9], [13, 10], [14, 12], [15, 23], [16, 18], [17, 24], [18, 21], [19, 13], [20, 15], [21, 16], [22, 17], [23, 20], [24, 22] |
| Op. 2 | 60.0° / [1 1 1] | [1, 3], [2, 8], [3, 1], [4, 9], [5, 6], [6, 5], [7, 14], [8, 2], [9, 4], [10, 15], [11, 12], [12, 11], [13, 23], [14, 7], [15, 10], [16, 17], [17, 16], [18, 22], [19, 20], [20, 19], [21, 24], [22, 18], [23, 13], [24, 21] |
| Op. 3 | 10.5° / [1 1 1] | [1, 4], [2, 10], [3, 9], [4, 1], [5, 16], [6, 17], [7, 18], [8, 15], [9, 3], [10, 2], [11, 13], [12, 23], [13, 11], [14, 22], [15, 8], [16, 5], [17, 6], [18, 7], [19, 21], [20, 24], [21, 19], [22, 14], [23, 12], [24, 20] |
| Op. 4 | 60.0° / [1 1 0] | [1, 2], [2, 5], [3, 6], [4, 7], [5, 1], [6, 8], [7, 11], [8, 3], [9, 12], [10, 13], [11, 4], [12, 14], [13, 19], [14, 9], [15, 20], [16, 21], [17, 22], [18, 16], [19, 10], [20, 23], [21, 18], [22, 24], [23, 15], [24, 17] |
| Op. 5 | 10.5° / [1 1 0] | [1, 6], [2, 3], [3, 2], [4, 12], [5, 8], [6, 1], [7, 9], [8, 5], [9, 7], [10, 20], [11, 14], [12, 4], [13, 15], [14, 11], [15, 13], [16, 22], [17, 21], [18, 24], [19, 23], [20, 10], [21, 17], [22, 16], [23, 19], [24, 18] |
| Op. 6 | 50.5° / [16 24 15] | [1, 16], [2, 4], [3, 15], [4, 13], [5, 10], [6, 9], [7, 1], [8, 17], [9, 22], [10, 21], [11, 18], [12, 3], [13, 2], [14, 23], [15, 12], [16, 7], [17, 20], [18, 19], [19, 11], [20, 8], [21, 5], [22, 6], [23, 24], [24, 14] |
| Op. 7 | 49.4° / [1 0 1] | [1, 8], [2, 6], [3, 5], [4, 14], [5, 3], [6, 2], [7, 12], [8, 1], [9, 11], [10, 23], [11, 9], [12, 7], [13, 20], [14, 4], [15, 19], [16, 24], [17, 18], [18, 17], [19, 15], [20, 13], [21, 22], [22, 21], [23, 10], [24, 16] |
| Op. 8 | 49.4° / [1 1 1] | [1, 9], [2, 15], [3, 4], [4, 3], [5, 17], [6, 16], [7, 22], [8, 10], [9, 1], [10, 8], [11, 23], [12, 13], [13, 12], [14, 18], [15, 2], [16, 6], [17, 5], [18, 14], [19, 24], [20, 21], [21, 20], [22, 7], [23, 11], [24, 19] |
| Op. 9 | 57.2° / [22 13 26] | [1, 11], [2, 19], [3, 14], [4, 5], [5, 18], [6, 24], [7, 21], [8, 23], [9, 8], [10, 1], [11, 10], [12, 20], [13, 7], [14, 17], [15, 6], [16, 2], [17, 3], [18, 4], [19, 16], [20, 22], [21, 13], [22, 12], [23, 9], [24, 15] |
| Op. 10 | 57.2° / [13 22 26] | [1, 10], [2, 16], [3, 17], [4, 18], [5, 4], [6, 15], [7, 13], [8, 9], [9, 23], [10, 11], [11, 1], [12, 22], [13, 21], [14, 3], [15, 24], [16, 19], [17, 14], [18, 5], [19, 2], [20, 12], [21, 7], [22, 20], [23, 8], [24, 6] |
| Op. 11 | 14.8° / [4 56 21] | [1, 17], [2, 9], [3, 10], [4, 23], [5, 15], [6, 4], [7, 3], [8, 16], [9, 18], [10, 24], [11, 22], [12, 1], [13, 8], [14, 13], [15, 11], [16, 14], [17, 19], [18, 20], [19, 12], [20, 2], [21, 6], [22, 5], [23, 21], [24, 7] |
| Op. 12 | 47.1° / [56 24 49] | [1, 18], [2, 11], [3, 23], [4, 10], [5, 19], [6, 14], [7, 5], [8, 24], [9, 17], [10, 16], [11, 21], [12, 8], [13, 1], [14, 20], [15, 9], [16, 4], [17, 15], [18, 13], [19, 7], [20, 6], [21, 2], [22, 3], [23, 22], [24, 12] |
| Op. 13 | 50.5° / [20 5 16] | [1, 15], [2, 17], [3, 16], [4, 22], [5, 9], [6, 10], [7, 23], [8, 4], [9, 13], [10, 12], [11, 3], [12, 18], [13, 24], [14, 1], [15, 21], [16, 20], [17, 7], [18, 6], [19, 8], [20, 11], [21, 14], [22, 19], [23, 2], [24, 5] |
| Op. 14 | 50.5° / [16 20 5] | [1, 14], [2, 23], [3, 11], [4, 8], [5, 24], [6, 18], [7, 17], [8, 19], [9, 5], [10, 6], [11, 20], [12, 10], [13, 9], [14, 21], [15, 1], [16, 3], [17, 2], [18, 12], [19, 22], [20, 16], [21, 15], [22, 4], [23, 7], [24, 13] |
| Op. 15 | 50.5° / [24 15 16] | [1, 7], [2, 13], [3, 12], [4, 2], [5, 21], [6, 22], [7, 16], [8, 20], [9, 6], [10, 5], [11, 19], [12, 15], [13, 4], [14, 24], [15, 3], [16, 1], [17, 8], [18, 11], [19, 18], [20, 17], [21, 10], [22, 9], [23, 14], [24, 23] |
| Op. 16 | 14.8° / [21 56 4] | [1, 12], [2, 20], [3, 7], [4, 6], [5, 22], [6, 21], [7, 24], [8, 13], [9, 2], [10, 3], [11, 15], [12, 19], [13, 14], [14, 16], [15, 5], [16, 8], [17, 1], [18, 9], [19, 17], [20, 18], [21, 23], [22, 11], [23, 4], [24, 10] |
| Op. 17 | 47.1° / [49 24 56] | [1, 13], [2, 21], [3, 22], [4, 16], [5, 7], [6, 20], [7, 19], [8, 12], [9, 15], [10, 4], [11, 2], [12, 24], [13, 18], [14, 6], [15, 17], [16, 10], [17, 9], [18, 1], [19, 5], [20, 14], [21, 11], [22, 23], [23, 3], [24, 8] |
| Op. 18 | 21.0° / [0 4 9] | [1, 19], [2, 18], [3, 24], [4, 21], [5, 11], [6, 23], [7, 10], [8, 14], [9, 20], [10, 7], [11, 5], [12, 17], [13, 16], [14, 8], [15, 22], [16, 13], [17, 12], [18, 2], [19, 1], [20, 9], [21, 4], [22, 15], [23, 6], [24, 3] |
| Op. 19 | 57.2° / [21 7 18] | [1, 24], [2, 14], [3, 19], [4, 20], [5, 23], [6, 11], [7, 8], [8, 18], [9, 21], [10, 22], [11, 17], [12, 5], [13, 6], [14, 10], [15, 7], [16, 12], [17, 13], [18, 15], [19, 9], [20, 1], [21, 3], [22, 2], [23, 16], [24, 4] |
| Op. 20 | 20.6° / [5 9 9] | [1, 21], [2, 7], [3, 20], [4, 19], [5, 13], [6, 12], [7, 2], [8, 22], [9, 24], [10, 18], [11, 16], [12, 6], [13, 5], [14, 15], [15, 14], [16, 11], [17, 23], [18, 10], [19, 4], [20, 3], [21, 1], [22, 8], [23, 17], [24, 9] |
| Op. 21 | 51.7° / [9 9 5] | [1, 22], [2, 12], [3, 13], [4, 15], [5, 20], [6, 7], [7, 6], [8, 21], [9, 16], [10, 17], [11, 24], [12, 2], [13, 3], [14, 19], [15, 4], [16, 9], [17, 10], [18, 23], [19, 14], [20, 5], [21, 8], [22, 1], [23, 18], [24, 11] |
| Op. 22 | 20.6° / [4 0 13] | [1, 23], [2, 24], [3, 18], [4, 17], [5, 14], [6, 19], [7, 20], [8, 11], [9, 10], [10, 9], [11, 8], [12, 21], [13, 22], [14, 5], [15, 16], [16, 15], [17, 4], [18, 3], [19, 6], [20, 7], [21, 12], [22, 13], [23, 1], [24, 2] |
| Op. 23 | 57.2° / [21 18 7] | [1, 20], [2, 22], [3, 21], [4, 24], [5, 12], [6, 13], [7, 15], [8, 7], [9, 19], [10, 14], [11, 6], [12, 16], [13, 17], [14, 2], [15, 18], [16, 23], [17, 11], [18, 8], [19, 3], [20, 4], [21, 9], [22, 10], [23, 5], [24, 1] |

*Table S3_2. Operators that link the KS variants, calculated by the software GenOVa. They are given by their index (first column), their angle/axis disorientation (second column) and the set of equivalent arrows, with [i,j] meaning the arrow from the variant $\alpha_i$ to the variant $\alpha_j$. The operators $O_3$ and $O_5$ have the lowest disorientation angle (10.5°) around [111]$\gamma$ and [110]$\gamma$, respectively. They are noted in the paper 2A and 2B respectively. Some operators are complementary polar operators such as $O_9$ - $O_{10}$, $Op_{13}$ - $O_{14}$, $O_{19}$ - $O_{23}$.*

# 2 The subgroupoids of KS variants

The CPD, CPP and Bain packets result from the classification of subsets of variants on crystallographic/ algebraic considerations; more explicitly, they correspond to subgroupoids of the groupoid of the 24 KS variants, without any consideration on the morphologies and habit planes. From Table S3_2, it can be noticed that there are two kinds of low-misoriented pairs of variants: the first pairs are variants linked by the operator $O_3$ = 10.5° / $[111]_\alpha$ that will be called 2A, and the second pairs are variants linked by the operator $O_5$ = 10.5° / $[110]_\alpha$ that will be called 2B. This last pairs form the blocks defined by Morito *et al.* (2003). The notation "2A" and "2B" come from the choice we made (and that is justified in the main paper) to name simply the rotation A(5.25°) = A and B(5.25°) = B. The three CPD, CPP and Bain crystallographic packets can then be built with the operators 2A, 2B and 2A+2B:

<u>CPD packets:</u> Some variants share a common $<111>_\alpha$ axis which is parallel to one $<110>_\gamma$ direction. It is possible to prove with the Table S3_2 and Table S3_1 that the sets of such variants and their operators form close assemblies, i.e. a subgroupoids. Since $<111>_\alpha$ and $<110>_\gamma$ axes are the dense directions of the respective phase, we will call those subgroupoids the Close Packed Direction (CPD) subgroupoids, or simply CPD packets. There are 6 CPD packets that each contains the operators $O_2$, $O_3$ and $O_8$. The CPD packets can be generated by one variant and two operators $O_2$ and $O_3$. They are explicitly given as sets of variants in Table S3_3.

| Name | Variants inside the packets | Operators inside the packets |
|---|---|---|
| CPD packets | CPD-1 = $\{\alpha_1, \alpha_3, \alpha_4, \alpha_9\}$<br>CPD-2 = $\{\alpha_2, \alpha_8, \alpha_{10}, \alpha_{15}\}$<br>CPD-3 = $\{\alpha_5, \alpha_6, \alpha_{16}, \alpha_{17}\}$<br>CPD-4 = $\{\alpha_7, \alpha_{14}, \alpha_{18}, \alpha_{22}\}$<br>CPD-5 = $\{\alpha_{11}, \alpha_{12}, \alpha_{13}, \alpha_{23}\}$<br>CPD-6 = $\{\alpha_{19}, \alpha_{20}, \alpha_{21}, \alpha_{24}\}$ | $\{O_0, O_2, O_3, O_8\}$ |
| CPP packets | CPP-1 = $\{\alpha_1, \alpha_2, \alpha_3, \alpha_5, \alpha_6, \alpha_8\}$<br>CPP-2 = $\{\alpha_4, \alpha_7, \alpha_9, \alpha_{11}, \alpha_{12}, \alpha_{14}\}$<br>CPP-3 = $\{\alpha_{10}, \alpha_{13}, \alpha_{15}, \alpha_{19}, \alpha_{20}, \alpha_{23}\}$<br>CPP-4 = $\{\alpha_{16}, \alpha_{17}, \alpha_{18}, \alpha_{21}, \alpha_{22}, \alpha_{24}\}$ | $\{O_0, O_1, O_2, O_4, O_5, O_7\}$ |
| Bain packets | Bain-1 = $\{\alpha_1, \alpha_4, \alpha_6, \alpha_{12}, \alpha_{17}, \alpha_{19}, \alpha_{21}, \alpha_{23}\}$<br>Bain-2 = $\{\alpha_5, \alpha_8, \alpha_{11}, \alpha_{13}, \alpha_{14}, \alpha_{15}, \alpha_{16}, \alpha_{22}\}$<br>Bain-3 = $\{\alpha_2, \alpha_3, \alpha_7, \alpha_9, \alpha_{10}, \alpha_{18}, \alpha_{20}, \alpha_{24}\}$ | $\{O_0, O_3, O_5, O_{11}, O_{16}, O_{18}, O_{20}, O_{22}\}$ |

*Table S3_3. Some important subgroupoids (packets) of KS variants: close packed direction (CPD), close packed plane (CPP) and Bain packets, with their sets of variants and operators.*

CPP packets: Some variants share a common $\{110\}_\alpha$ plane which is parallel to one $\{111\}_\gamma$ plane. Even if obvious geometrically, here again it can be proved that the sets of such assemblies of variants are close under the groupoid actions and are therefore subgroupoids. Since $\{110\}_\alpha$ and $\{111\}_\gamma$ planes are the dense planes of the respective phase, we will call those subgroupoids the Close Packed Plane (CPP) subgroupoids, or simply CPP packets. There are 4 CPP packets that each contains the operators $O_1$, $O_2$, $O_4$, $O_5$ and $O_7$. The CPP packets can be generated by one variant and two operators $O_1$ and $O_5$. They correspond to the "packets" defined by Morito *et al.* (2003). They are given as sets of variants in Table S3_3.

Bain packets: Some variants are linked between them by low misorientations. They are the crystallographic packets defined by Gourgues *et al.* (2000), also called Bain zones. The two lowest misorientations are the 2A and 2B operators, i.e. $O_3$ = 10.5° / $[111]_\alpha$ and $O_5$ = 10.5° / $[110]_\alpha$. May the structure, generated by one variant and these two operators, be really closed? Would it not form the whole groupoid of 24 KS variants? The solution is not obvious geometrically (at least at first thought). Let's consider the variant $\alpha_1$ and build the other variants generated by the operators 2A and 2B. The result is given graphically in Fig. S3_2. The set of generated variants is indeed closed and contains 8 variants. Therefore there are 3 Bain packets. Each packet forms in the $<100>_\alpha$ pole figures a Bain circle around one of the three $<100>_\gamma$ directions. They are given as sets of variants in Table S3_3.

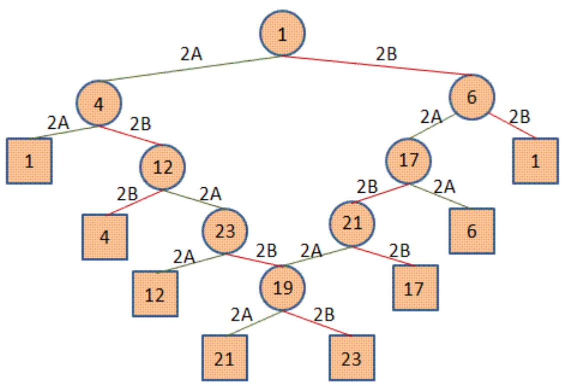


*Fig. S3_2. A Bain packet in a tree form. This subgroupoid is generated by the variant $\alpha_1$ and the two low-misorientation operators 2A= $O_3$ and 2B = $O_5$. The numbers in the circles are the indexes of the KS variants. The tree is stopped when the variants generated by 2A and 2B are those already created by the previous steps (noted by the squares).*

The method used to build the CPD, CPP and Bain packets in steels is actually general and can be applied to define packets of variants for any structural phase transformation.