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# A theoretical investigation of orientation relationships and transformation strains in steels

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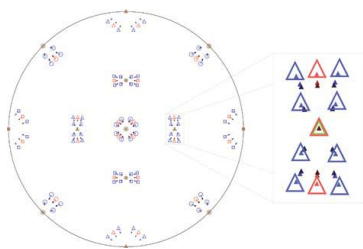
**Keywords:** orientation relationships; Nishiyama–Wassermann; Kurdjumov–Sachs; Pitsch; Greninger–Troiano; Bain; inverse Greninger–Troiano; steel; ratio of tetragonality; transformation strains; f.c.c. to b.c.c. transformations; f.c.c. to b.c.t. transformations.

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The identification of orientation relationships (ORs) plays a crucial role in the understanding of solid phase transformations. In steels, the most common models of ORs are the ones by Nishiyama–Wassermann (NW) and Kurdjumov–Sachs (KS). The defining feature of these and other OR models is the matching of directions and planes in the parent face-centred cubic  $\gamma$  phase to ones in the product body-centred cubic/tetragonal  $\alpha/\alpha'$  phase. In this article a novel method that identifies transformation strains with ORs is introduced and used to develop a new strain-based approach to phase-transformation models in steels. Using this approach, it is shown that the transformation strains that leave a close-packed plane in the  $\gamma$  phase and a close-packed direction within that plane unrotated are precisely those giving rise to the NW and KS ORs when a cubic product phase is considered. Further, it is outlined how, by choosing different pairs of unrotated planes and directions, other common ORs such as the ones by Pitsch and Greninger–Troiano can be derived. One of the advantages of our approach is that it leads to a natural generalization of the NW, KS and other ORs for different ratios of tetragonality  $r$  of the product body-centred tetragonal  $\alpha'$  phase. These generalized ORs predict a sharpening of the transformation textures with increasing tetragonality and are thus in qualitative agreement with experiments on steels with varying alloy concentration.

## 1. Introduction

The transformation mechanism from the face-centred cubic (f.c.c.) to the body-centred cubic/tetragonal (b.c.c./b.c.t.) phase of steel has received widespread attention and the most influential early studies include those of Bain (1924), Kurdjumov & Sachs (1930), Nishiyama (1934) and Wassermann (1935). In his seminal paper, Bain (1924) proposed a mechanism that transforms the f.c.c.  $\gamma$  phase of iron to its b.c.c.  $\alpha$  phase ‘requiring the least temporary distortion’. His conceived mechanism, although now widely accepted, was not without criticism from his contemporaries. Among the critics were Kurdjumov and Sachs (Kurdjumov & Sachs, 1930) who conducted X-ray diffraction measurements on 1.4% carbon steel and measured the orientation relationships between austenite and pure b.c.c.  $\alpha$  iron as well as between austenite and 1.4% C  $\alpha'$  steel.<sup>1</sup> The most important feature of their mechanism was the parallelism between the  $(111)_\gamma$  and the  $(011)_{\alpha'}$  plane as well as the  $[10\bar{1}]_\gamma$  and the  $[1\bar{1}1]_{\alpha'}$  direction, and they explained how these conditions can be satisfied by a combination of three shears. Following their construction step by step, one sees that the overall deformation is always one of the Bain strains followed by a rigid-body rotation and that the



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<sup>1</sup> Henceforth, we adopt the convention from Nishiyama (1978) of using the symbol  $\alpha'$  for the low-temperature phase of steels irrespectively of whether it is cubic or tetragonal.

resulting orientation relationship for pure iron differs from the one for 1.4% C steel [see Tables 2 in Kurdjumov & Sachs (1930) and Otte (1960)]. Using the same methods, Nishiyama (1934) investigated an Fe–30% Ni single crystal which, like pure iron, undergoes an f.c.c. to b.c.c. transformation. Based on his observations, Nishiyama proposed a different orientation relationship that has the same parallel planes but the direction  $[10\bar{1}]_\gamma$  parallel to  $[100]_\alpha$ . One year later, Wassermann (1935) independently postulated the same relationships and also confirmed the earlier results by Kurdjumov and Sachs. Apart from the Nishiyama–Wassermann (NW) and Kurdjumov–Sachs (KS) orientation relationships (ORs) several other ORs, *e.g.* by Pitsch (1959) (P) and Greninger–Troiano (Greninger & Troiano, 1949) (GT), have been proposed and they all share the common feature of matching directions and planes in the parent phase to ones in the product phase.

Apart from ORs, an equally important notion in the modelling of solid phase transitions is the transformation strain. Nevertheless, a clear connection between the two notions is missing. In the context of the crystallographic theory of martensite, ORs are deduced from strains in order to compare theoretical predictions with experiments (Christian, 2002; Khachaturyan, 2013). For the more challenging reverse direction, attempts have been made (see *e.g.* Bollmann, 1974; Guo *et al.*, 2004) to deduce transformation strains from a given OR. However, these attempts seem to be missing a general and systematic method, in turn leading to inconsistencies in the obtained strains.

In the present article, we would like to introduce a systematic and conceptually clear approach to ORs and transformation strains in steels. Compared to the aforementioned works as well as *e.g.* Cayron *et al.* (2010) and He *et al.* (2005), this approach brings the following novelties:

(i) The only necessary inputs are the lattice parameters of the two phases and the knowledge of a plane and a direction that are left unrotated.

(ii) It shows that the notions of transformation strains and ORs are equivalent. That is, for any given strain a corresponding OR can be calculated and the parallelisms between planes and directions in the two phases follow. Conversely, given such an OR the method uniquely retrieves the strain that gave rise to it.

(iii) The additional knowledge of the actual underlying deformation of the material can *e.g.* be used to unambiguously determine twin relationships (*cf.* §2.2) and generally lay the groundwork for mathematical theories of steels based on energy minimization (see *e.g.* Bhattacharya, 2003; Koumatos & Muehleemann, 2015).

(iv) Our method takes into account the ratio of tetragonality  $r = c/a$  of the b.c.t.  $\alpha'$  phase. Thus, the derived strains and ORs also depend on  $r$  and can be expressed explicitly as functions of  $r$ .

For  $r = 1$ , corresponding to b.c.c., we recover the original NW, KS and P ORs. However, for  $r > 1$ , our approach predicts a deviation from the original ORs. We show how this leads to a sharpening of the transformation textures and how it can be

used to explain the deviation from the exact parallelism condition in the GT ORs.

The structure of the paper is as follows: at the end of this section we clarify the notation that will be used throughout. In §2, we introduce a unified approach for the derivation of phase-transformation models in steels, which entails a general method to identify transformation strains with ORs. In §3, we apply our unified approach to deduce the KS and NW transformation strains and ORs; we also comment on how the obtained ORs relate to other common descriptions of the NW and KS ORs and show how the additional knowledge of the strains can be used to unambiguously determine twin relationships between KS variants. At the end of §3, we illustrate how according to our unified approach the KS and NW ORs change with increasing ratio of tetragonality  $r$  of the  $\alpha'$  phase. In §4, we indicate how the same methods can be used to explain and generalize the P, GT and inverse Greninger–Troiano (GT') OR models.

### 1.1. Preliminaries

Let us consider an orthonormal basis  $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$ . By  $[abc] = (a\mathbf{f}_1 + b\mathbf{f}_2 + c\mathbf{f}_3)/(a^2 + b^2 + c^2)^{1/2}$  we denote a normalized direction expressed in this basis.<sup>2</sup> Similarly, by  $(abc)$  we denote a normal in the same basis.<sup>3</sup> For  $\mathbf{u} = [u_1 u_2 u_3]$  and  $\mathbf{v} = [v_1 v_2 v_3]$  we denote by  $\mathbf{u} \cdot \mathbf{v}$  the inner product, by  $|\mathbf{u}|$  the norm and by  $\mathbf{u} \times \mathbf{v}$  the cross product. That is  $\mathbf{u} \cdot \mathbf{v} = u_1v_1 + u_2v_2 + u_3v_3$ ,  $|\mathbf{u}| = (\mathbf{u} \cdot \mathbf{u})^{1/2}$  and  $\mathbf{u} \times \mathbf{v} = (u_2v_3 - u_3v_2)\mathbf{f}_1 + (u_3v_1 - u_1v_3)\mathbf{f}_2 + (u_1v_2 - u_2v_1)\mathbf{f}_3$ . We also recall the identities

$$(\mathbf{m} \times \mathbf{u}) \cdot (\mathbf{n} \times \mathbf{v}) = (\mathbf{m} \cdot \mathbf{n})(\mathbf{u} \cdot \mathbf{v}) - (\mathbf{u} \cdot \mathbf{n})(\mathbf{v} \cdot \mathbf{m}) \quad (1)$$

and

$$A\mathbf{u} \times A\mathbf{v} = \text{cof } A(\mathbf{u} \times \mathbf{v}), \quad (2)$$

where  $A$  is a  $3 \times 3$  matrix. In particular, the matrix of cofactors,  $\text{cof } A$ , measures how a vector normal to  $\mathbf{u}$  and  $\mathbf{v}$  deforms whenever  $\mathbf{u}$  and  $\mathbf{v}$  are deformed by  $A$ . If  $A$  is invertible it holds that  $\text{cof } A = A^{-T} \det A$ , where as usual  $A^{-T}$  denotes the inverse of the transpose.

We end this section by summarizing some important properties of rotation matrices, *i.e.*  $3 \times 3$  matrices  $R$  such that  $R^T R = \mathbb{I}$  and  $\det R = 1$ . Any rotation matrix  $R$  can be uniquely identified as a counterclockwise rotation by an angle  $\phi$  about a vector  $\mathbf{u}$  and we write  $R = R[\phi, \mathbf{u}]$ , where  $\mathbf{u}$  is always expressed in the standard basis  $\mathbf{e}_1 = (1, 0, 0)^T$ ,  $\mathbf{e}_2 = (0, 1, 0)^T$ ,  $\mathbf{e}_3 = (0, 0, 1)^T$ . The magnitude of the angle of rotation is given by  $|\phi| = \arccos((\text{Tr } R - 1)/2)$ , where  $\text{Tr } R = \sum_{i=1}^3 R_{ii}$  is the trace of the matrix  $R$  and the sign of  $\phi$  is given by  $\text{sgn}(\phi) = \text{sgn}((\mathbf{n} \times R\mathbf{n}) \cdot \mathbf{u})$ , where  $\mathbf{n}$  is any vector that is not parallel to the axis of rotation  $\mathbf{u}$ . In particular, reversing the sign of the axis  $\mathbf{u} \rightarrow -\mathbf{u}$  is equivalent to reversing the sign of the angle of rotation  $\phi \rightarrow -\phi$ . Finally, by  $\mathcal{P}^{24}$  we denote the group of rotations that map a cube to itself (see the supporting

<sup>2</sup> As is commonly asserted in the literature, we make the identification  $-a = \bar{a}$ .

<sup>3</sup> Note that since  $\{\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3\}$  is an orthonormal basis it coincides with its reciprocal basis, *i.e.*  $[abc] = (abc)$ .

information) and we call two vectors  $\mathbf{n}, \mathbf{n}'$  crystallographically equivalent iff  $\mathbf{n}' = P\mathbf{n}$  for some  $P \in \mathcal{P}^{24}$ .

## 2. A unified approach to phase transformation models in steels

Since Bain's seminal paper (Bain, 1924) [see also Koumatos & Muehleemann (2016) for a rigorous mathematical justification] it is well known that the pure stretches required to transform an f.c.c. lattice to a b.c.c./b.c.t. lattice are given by the three Bain strains:

$$B_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}, B_2 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}, B_3 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}, \quad (3)$$

where  $\alpha = (2^{1/2}a)/a_0$  and  $\beta = c/a_0$ . Here  $a_0$  is the lattice parameter of the f.c.c. phase and  $c \geq a$  are the lattice parameters of the b.c.t. phase ( $a = c$  for b.c.c.). An additional rigid-body rotation  $R$  does not change the b.c.c./b.c.t. lattice structure and hence any lattice transformation  $T$  from f.c.c. to b.c.c./b.c.t. is of the form

$$T = RB_i \text{ for some } i = 1, 2, 3.$$

Now, suppose that the transformation  $T$  leaves a plane with normal  $\mathbf{n}$  and a direction  $\mathbf{v}$  within that plane unrotated, i.e.

$$\frac{\text{cof } T \mathbf{n}}{|\text{cof } T \mathbf{n}|} = R \frac{\text{cof } B_i \mathbf{n}}{|\text{cof } B_i \mathbf{n}|} = \mathbf{n} \text{ and } \frac{T \mathbf{v}}{|T \mathbf{v}|} = R \frac{B_i \mathbf{v}}{|B_i \mathbf{v}|} = \mathbf{v}. \quad (4)$$

Defining  $\mathbf{m}_i = \text{cof } B_i \mathbf{n} / |\text{cof } B_i \mathbf{n}|$ ,  $\mathbf{u}_i = B_i \mathbf{v} / |B_i \mathbf{v}|$ , we observe that<sup>4</sup>

$$\mathbf{m}_i \cdot \mathbf{u}_i \propto \text{cof } B_i \mathbf{n} \cdot B_i \mathbf{v} = B_i^T \text{cof } B_i \mathbf{n} \cdot \mathbf{v} \propto \mathbf{n} \cdot \mathbf{v} = 0,$$

where we have used that  $\text{cof } B_i \propto B_i^{-T}$  and that  $\mathbf{v} \perp \mathbf{n}$ . In particular, the pairs  $\mathbf{m}_i, \mathbf{u}_i$  and  $\mathbf{n}, \mathbf{v}$  are both orthonormal and thus there is a unique rotation  $R = R_i$  such that  $R_i \mathbf{m}_i = \mathbf{n}$  and  $R_i \mathbf{u}_i = \mathbf{v}$  given by

$$R_i = \begin{pmatrix} | & | & | \\ \mathbf{n} & \mathbf{v} & \mathbf{n} \times \mathbf{v} \\ | & | & | \end{pmatrix} \begin{pmatrix} - & \mathbf{m}_i & - \\ - & \mathbf{u}_i & - \\ - & \mathbf{m}_i \times \mathbf{u}_i & - \end{pmatrix}. \quad (5)$$

Consequently, for each  $i = 1, 2, 3$  there is exactly one transformation strain,  $T_i = R_i B_i$ , from f.c.c. to b.c.c./b.c.t. that leaves the plane with normal  $\mathbf{n}$  and the direction  $\mathbf{v}$  within that plane unrotated.

### 2.1. Identifying strains with orientation relationships

Given the transformation strain  $T_i$ , we show how to compute the corresponding OR. For simplicity, we focus on the case  $i = 2$ ; the remaining two cases can be treated analogously. From the pure Bain mechanism it is clear that the transformation  $B_2$  results in a b.c.c./b.c.t. unit cell with edges along the directions  $\mathbf{e}_1 - \mathbf{e}_3$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_1 + \mathbf{e}_3$  (see Fig. 1). The

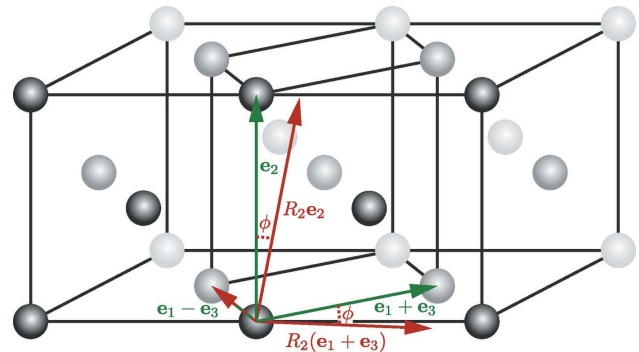


Figure 1  
The green vectors  $\mathbf{e}_1 - \mathbf{e}_3, \mathbf{e}_2, \mathbf{e}_1 + \mathbf{e}_3$  are along the edges of the tetragonal b.c.t. cell that is contained in the f.c.c. lattice and the red vectors are obtained through the rotation  $R_2$ .

additional rotation  $R_2$  in the transformation  $T_2$  then results in a b.c.c./b.c.t. unit cell with edges along the directions

$$R_2(\mathbf{e}_1 - \mathbf{e}_3), R_2 \mathbf{e}_2 \text{ and } R_2(\mathbf{e}_1 + \mathbf{e}_3),$$

which form the natural basis for the b.c.c./b.c.t. lattice.

Noting that  $\mathbf{e}_1 - \mathbf{e}_3 = R[45^\circ, \mathbf{e}_2] \mathbf{e}_1$  and  $\mathbf{e}_1 + \mathbf{e}_3 = R[45^\circ, \mathbf{e}_2] \mathbf{e}_3$  we see that the change of basis matrix between f.c.c. and b.c.c./b.c.t. is given by  $R_2 R[45^\circ, \mathbf{e}_2]$ , i.e.  $\mathbf{x} = [x_1 \ x_2 \ x_3]_\gamma = [\hat{x}_1 \ \hat{x}_2 \ \hat{x}_3]_{\alpha'}$ , where

$$\begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \hat{x}_3 \end{pmatrix} = R[-45^\circ, \mathbf{e}_2] R_2^T \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} =: O_2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \quad (6)$$

In particular, through the matrix  $O_2 = R[-45^\circ, \mathbf{e}_2] R_2^T$  one can express the coordinates of the unrotated plane  $\mathbf{n}$  and direction  $\mathbf{v}$  in the new b.c.c./b.c.t. ( $\alpha'$ ) basis and hence determine the orientation relationship. In general, the OR corresponding to  $T_i = R_i B_i$  is given through the matrix

$$O_i = R[-45^\circ, \mathbf{e}_i] R_i^T, \quad (7)$$

which we henceforth call the orientation relationship matrix. We note that  $R[45^\circ, \mathbf{e}_i] = R[90^\circ, \mathbf{e}_i] R[-45^\circ, \mathbf{e}_i]$  with  $R[90^\circ, \mathbf{e}_i] \in \mathcal{P}^{24}$ , i.e. choosing the opposite sign for the 45° rotation about  $\mathbf{e}_i$  simply leads to a crystallographically equivalent normal and direction. In summary, starting from the transformation  $T_i$ , we obtain the orientation relationship

$$(n_1 \ n_2 \ n_3)_\gamma \parallel (\hat{n}_1 \ \hat{n}_2 \ \hat{n}_3)_{\alpha'} \text{ and } [v_1 \ v_2 \ v_3]_\gamma \parallel [\hat{v}_1 \ \hat{v}_2 \ \hat{v}_3]_{\alpha'}, \quad (8)$$

where the coordinates  $\hat{n}_i$  and  $\hat{v}_i$  are obtained by using the orientation relationship matrix  $O_i$  from (7) in (6).

Conversely, suppose that an OR of the form (8) is given with the property that the normal  $(n_1 \ n_2 \ n_3)_\gamma$  and the direction  $[v_1 \ v_2 \ v_3]_\gamma$  are left unrotated by the transformation. By the above process, we can compute three possible transformation strains  $T_i$  and corresponding OR matrices  $O_i$ . For each OR matrix  $O_i$  we can calculate the b.c.c./b.c.t. coordinates of  $(n_1 \ n_2 \ n_3)_\gamma$  and  $[v_1 \ v_2 \ v_3]_\gamma$ . For one of the matrices  $O_i$ , the calculated coordinates must agree, up to crystallographic equivalence, with the given OR and, hence, we may uniquely identify the Bain variant  $B_i$ , and the corresponding transfor-

<sup>4</sup> Recall that  $x \propto y$  if there is a constant  $c$  such that  $x = cy$ .

**Table 1**  
The NW orientation relationships.

The corresponding variants in each row are given by  $T_{NWj} = R[\phi(r), \mathbf{v}_j]B_j$ .

OR†	f.c.c. plane‡	b.c.c. plane	f.c.c. direction§	b.c.c. direction	Bain variant¶
NW1	$(111)_\gamma$	$(011)_{\alpha'}$	$[10\bar{1}]_\gamma$	$[100]_{\alpha'}$	$B_2$
NW2	$(111)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}10]_\gamma$	$[100]_{\alpha'}$	$B_3$
NW3	$(111)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[100]_{\alpha'}$	$B_1$
NW4	$(\bar{1}\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[101]_\gamma$	$[100]_{\alpha'}$	$B_2$
NW5	$(\bar{1}\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[\bar{1}\bar{1}0]_\gamma$	$[100]_{\alpha'}$	$B_3$
NW6	$(\bar{1}\bar{1}1)_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[100]_{\alpha'}$	$B_1$
NW7	$(1\bar{1}\bar{1})_\gamma$	$(011)_{\alpha'}$	$[\bar{1}01]_\gamma$	$[100]_{\alpha'}$	$B_2$
NW8	$(1\bar{1}\bar{1})_\gamma$	$(011)_{\alpha'}$	$[110]_\gamma$	$[100]_{\alpha'}$	$B_3$
NW9	$(1\bar{1}\bar{1})_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}\bar{1}]_\gamma$	$[100]_{\alpha'}$	$B_1$
NW10	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[\bar{1}0\bar{1}]_\gamma$	$[100]_{\alpha'}$	$B_2$
NW11	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[1\bar{1}0]_\gamma$	$[100]_{\alpha'}$	$B_3$
NW12	$(11\bar{1})_\gamma$	$(011)_{\alpha'}$	$[0\bar{1}1]_\gamma$	$[100]_{\alpha'}$	$B_1$

† NWj. ‡  $P_{2j-1}(111)_\gamma$ . §  $\mathbf{v}_j = P_{2j-1}[10\bar{1}]_\gamma$ . ¶  $B_j = P_{2j-1}B_2P_{2j-1}^T$ .

mation strain  $T_i$ , that give rise to the OR. If the coordinates do not agree for any  $O_i$ , then the OR cannot be compatible with the Bain mechanism.

### 2.2. Generating variants through crystallographic equivalence in the $\gamma$ phase

Given a transformation strain  $T$  (or equivalently the corresponding OR matrix  $O$ ) we are able to generate further variants of  $T$  through the application of  $\mathcal{P}^{24}$  in the reference configuration. To this end, we recall that given the f.c.c. basis  $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ , all crystallographically equivalent f.c.c. bases are given by  $\{P\mathbf{e}_1, P\mathbf{e}_2, P\mathbf{e}_3\}$  for  $P \in \mathcal{P}^{24}$ . Thus, setting  $T$  as in (4) and using the identity  $P_i^T P_i = \mathbb{I}$ , we infer that

$$\frac{\text{cof}(P_i T P_i^T) P_i \mathbf{n}}{|\text{cof } T \mathbf{n}|} = P_i \mathbf{n} \text{ and } \frac{(P_i T P_i^T) P_i \mathbf{v}}{|T \mathbf{v}|} = P_i \mathbf{v}.$$

That is, for each  $i = 1, 2, \dots, 24$ , the deformation  $P_i T P_i^T$  leaves the plane with normal  $P_i \mathbf{n}$  and the direction  $P_i \mathbf{v}$  within that plane unrotated and thus describes a *strain variant* of the original transformation strain  $T$ . Similarly,  $P_i O P_i^T$  describes the corresponding *orientation relationship variant*. We note that, in general, it may happen (see e.g. the NW model) that  $P_i T P_i^T = P_j T P_j^T$  for some  $i \neq j$  and thus there can be less than 24 distinct variants for a given transformation strain (or equivalently for a given OR).

### 3. The NW and KS models

In this section, we derive the NW and KS models. Both models have the attractive feature of leaving a close-packed  $\{111\}_\gamma$  plane and a close-packed  $\langle \bar{1}10 \rangle$  direction within that plane unrotated. Owing to this feature they seem to be the most natural candidates for OR models. To carry out the derivation we apply our unified approach from §2 with

$$\mathbf{n} = (111)_\gamma \text{ and } \mathbf{v} = [10\bar{1}]_\gamma.$$

### 3.1. The transformation with stretch component $B_2$

Let us consider the second Bain variant  $B_2$ . Noting that  $\mathbf{v}$  is an eigenvector of  $B_2$ , we immediately deduce that, by (4),  $R_2 \mathbf{v} = \mathbf{v}$  and thus  $\mathbf{v}$  is the axis of rotation. Regarding the angle of rotation we calculate

$$\text{Tr } R_2 = \mathbf{m}_2 \cdot \mathbf{n} + \mathbf{u}_2 \cdot \mathbf{v} + (\mathbf{m}_2 \times \mathbf{u}_2) \cdot (\mathbf{n} \times \mathbf{v}) = 2\mathbf{m}_2 \cdot \mathbf{n} + 1,$$

where we use that  $\mathbf{u}_2 = \mathbf{v}$  and (1). Hence, the angle of rotation is given by

$$\begin{aligned} & \arccos\left(\frac{\text{cof } B_2 \mathbf{n} \cdot \mathbf{n}}{|\text{cof } B_2 \mathbf{n}|}\right) \text{sgn}((\mathbf{m}_2 \times \mathbf{n}) \cdot \mathbf{v}) \\ &= \arccos\left(\frac{1 + 2^{1/2}r}{3^{1/2}(1+r^2)^{1/2}}\right) =: \phi(r), \end{aligned} \quad (9)$$

where  $r = c/a = 2^{1/2}\beta/\alpha$  is the ratio of tetragonality of the b.c.t. cell. In particular, for  $r = 1$  corresponding to a b.c.c. product lattice we obtain  $\phi(1) = \arccos[(1 + 2^{1/2})/6^{1/2}] \simeq 9.7356^\circ$ .

Hence, the only transformation from f.c.c. to b.c.c./b.c.t. with stretch component  $B_2$  which leaves the plane  $(111)_\gamma$  and the direction  $[10\bar{1}]_\gamma$  unrotated is

$$T_2 = R_2 B_2 = R[\phi(r), [10\bar{1}]]B_2. \quad (10)$$

Regarding the ORs corresponding to  $T_2$ , through (10) and (7), we infer that  $O_2 = R[-45^\circ, \mathbf{e}_2]R[-\phi(r), [10\bar{1}]]$  (cf. Fig. 1). Consequently,

$$(111)_\gamma \parallel (01r)_{\alpha'} \text{ and } [10\bar{1}]_\gamma \parallel [100]_{\alpha'}. \quad (11)$$

Note that, as expected, the latter is a closest-packed plane in the resulting b.c.t. lattice containing the b.c.t. direction  $[100]_{\alpha'}$ . Thus, for  $r = 1$  (b.c.c.) the transformation  $T_2$  gives rise to the OR NW1 (see Table 1) and henceforth we denote  $T_2 = T_{NW1}$ . The OR matrix  $O_{NW1}$  between f.c.c. and b.c.c. is given by

$$\begin{aligned} O_{NW1} &= R[-45^\circ, \mathbf{e}_2]R[-9.7356^\circ, [10\bar{1}]] \\ &\simeq \begin{pmatrix} 0.7071 & 0 & -0.7071 \\ 0.1196 & 0.9856 & 0.1196 \\ 0.6969 & -0.1691 & 0.6969 \end{pmatrix}, \end{aligned}$$

and the corresponding transformation  $T_{NW1}$  is given by

$$\begin{aligned} T_{NW1} &= R[9.7356^\circ, [10\bar{1}]]B_2 \\ &\simeq \begin{pmatrix} 1.1144 & 0.0949 & -0.0081 \\ -0.1342 & 0.7823 & -0.1342 \\ -0.0081 & 0.0949 & 1.1144 \end{pmatrix}. \end{aligned}$$

Next, we characterize the remaining NW variants. Following our unified approach, they are given by  $P_i T_{NW1} P_i^T$ . Since  $T_{NW1} = R[\phi(r), [10\bar{1}]]B_2$ ,  $P_2[10\bar{1}]_\gamma = [10\bar{1}]_\gamma$  and  $P_2 B_2 P_2^T = B_2$  we deduce that  $P_2 T_{NW1} P_2^T = T_{NW1}$  and similarly that  $P_{2j} T_{NW1} P_{2j}^T = P_{2j-1} T_{NW1} P_{2j-1}^T$  for any  $j = 2, \dots, 12$ . Thus, there are only 12 NW strain variants given by

$$T_{NWj} := P_{2j-1} T_{NW1} P_{2j-1}^T = R[\phi(r), P_{2j-1}[10\bar{1}]]P_{2j-1} B_2 P_{2j-1}^T,$$

for  $j = 1, 2, \dots, 12$ . In particular,  $T_{NWj}$  has a stretch component  $P_{2j-1} B_2 P_{2j-1}^T$  followed by a rotation of  $\phi(r)$  about

**Table 2**  
The KS orientation relationships.

The corresponding variants in each row are given by  $T_{KSj} = R[(-1)^{j+1}\theta(r), \mathbf{n}_j]R[\phi(r), P_j[\bar{1}10]]B_j$ .

OR†	f.c.c. plane‡	b.c.c. plane	f.c.c. direction§	b.c.c. direction	Bain variant¶
KS1	(111) <sub>y</sub>	(011) <sub>α'</sub>	[10 $\bar{1}$ ] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS2	(111) <sub>y</sub>	(011) <sub>α'</sub>	[10 $\bar{1}$ ] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS3	(111) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 10] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS4	(111) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 10] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS5	(111) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS6	(111) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS7	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[101] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS8	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[101] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS9	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 10] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS10	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 10] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS11	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS12	( $\bar{1}$ 11) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS13	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 01] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS14	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 01] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS15	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[110] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS16	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[110] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS17	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS18	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[0 $\bar{1}$ 1] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS19	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 0 $\bar{1}$ ] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS20	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[ $\bar{1}$ 0 $\bar{1}$ ] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS21	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[1 $\bar{1}$ 0] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>
KS22	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[1 $\bar{1}$ 0] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>1</sub>
KS23	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[011] <sub>y</sub>	[11 $\bar{1}$ ] <sub>α'</sub>	B <sub>3</sub>
KS24	(1 $\bar{1}$ 1) <sub>y</sub>	(011) <sub>α'</sub>	[011] <sub>y</sub>	[ $\bar{1}$ 1 $\bar{1}$ ] <sub>α'</sub>	B <sub>2</sub>

† KS<sub>j</sub>. ‡  $\mathbf{n}_j = (-1)^{j+1}P_j(111)_y$ . §  $P_j[10\bar{1}]_y$ . ¶  $B_j = P_jB_3P_j^T$ .

$P_{2j-1}[10\bar{1}]_y$ . The corresponding OR matrices are obtained by the same conjugation. That is

$$O_{NWj} = P_{2j-1}O_{NW1}P_{2j-1}^T = R[-45^\circ, P_{2j-1}\mathbf{e}_2]R[-\phi(r), P_{2j-1}[10\bar{1}]]$$

for  $j = 1, 2, \dots, 12$ . Thus, by (11),  $O_{NWj}$  maps the f.c.c. normal  $P_{2j-1}\mathbf{n}$  and f.c.c. vector  $P_{2j-1}\mathbf{v}$  to the b.c.c./b.c.t. normal  $P_{2j-1}(01r)_{\alpha'}$  and the b.c.c./b.c.t. direction  $P_{2j-1}[100]_{\alpha'}$  (see Table A1 in the supporting information). It is easy to verify that, for  $r = 1$ , the resulting b.c.c. vectors are crystallographically equivalent (through  $P_{2j-1}^T$ ) to the b.c.c. vector  $[100]_{\alpha'}$  and the b.c.c. normal  $(011)_{\alpha'}$ , giving the NW variants as in Table 1. We note that the choice of sign for the  $45^\circ$  rotation about  $\mathbf{e}_2$ , as well as the enumeration of  $\mathcal{P}^{24}$ , has been carefully made so that the OR NW<sub>j</sub> is obtained through  $P_{2j-1}^T$ . A choice of the opposite sign and/or a different enumeration of  $\mathcal{P}^{24}$  will not alter the result but will lead to b.c.c./b.c.t. coordinates that are crystallographically equivalent to the ones in Table 1 through different elements of  $\mathcal{P}^{24}$ .

### 3.2. The transformation with stretch component B<sub>3</sub>

Similarly, using  $B_3$  instead of  $B_2$  in (4) gives rise to a rotation  $R_3$  satisfying

$$R_3\mathbf{m}_3 = \mathbf{n} \text{ and } R_3\mathbf{u}_3 = \mathbf{v}. \quad (12)$$

Noting that  $R_{NW2}\mathbf{m}_3 = \mathbf{n}$  we immediately see that  $R_3R_{NW2}^T\mathbf{n} = \mathbf{n}$  and

$$R_3 = R[\theta, \mathbf{n}]R_{NW2} = R[\theta, [111]]R[\phi(r), [\bar{1}10]]$$

for some angle  $\theta = \theta(r)$ . Let us first determine the sign of  $\theta(r)$ . By (12), we have that  $R[\theta, \mathbf{n}]R_{NW2}\mathbf{u}_3 = \mathbf{v}$  and thus  $\text{sgn } \theta(r) = \text{sgn}(R_{NW2}\mathbf{u}_3 \times \mathbf{v}) \cdot \mathbf{n} = 1$ . For the angle itself we deduce from (5) that

$$\theta(r) = \arccos\left(\frac{\text{Tr } R[\theta, \mathbf{n}] - 1}{2}\right) = \arccos\left(\frac{3^{1/2}(r^2 + 1)^{1/2} + 1}{2(r^2 + 2)^{1/2}}\right). \quad (13)$$

For  $r = 1$  (b.c.c.) this angle is given by  $\theta(1) = \arccos[(1 + 6^{1/2})/(2(3)^{1/2})] \simeq 5.2644^\circ$ . Hence, the only transformation from f.c.c. to b.c.c./b.c.t. with stretch component  $B_3$  which leaves the plane  $(111)_y$  and the direction  $[10\bar{1}]_y$  unrotated is

$$T_3 = R_3B_3 = R[\theta(r), [111]]R[\phi(r), [\bar{1}10]]B_3. \quad (14)$$

Regarding the corresponding ORs, by (7) we deduce that

$$O_3 = R[45^\circ, \mathbf{e}_3]R[-\phi(r), [\bar{1}10]]R[-\theta(r), [111]] \quad (15)$$

and, consequently,

$$(111)_y \parallel (0r1)_{\alpha'} \text{ and } [10\bar{1}]_y \parallel [11\bar{r}]_{\alpha'}. \quad (16)$$

In particular, the resulting  $\alpha'$  normal is a closest-packed plane in the b.c.c./b.c.t. lattice and the resulting  $\alpha'$  direction is a close-packed direction within that plane. Clearly, for  $r = 1$  (b.c.c.), the transformation  $T_3$  gives rise to the OR KS1 (see Table 2) and henceforth we denote  $T_3 = T_{KS1}$ . The OR matrix  $O_{KS1}$  between f.c.c. and b.c.c. is then given by

$$O_{KS1} = R[45^\circ, \mathbf{e}_3]R[-9.7356^\circ, [\bar{1}10]]R[-5.2644^\circ, [111]] \simeq \begin{pmatrix} 0.7416 & -0.6667 & -0.0749 \\ 0.6498 & 0.7416 & -0.1667 \\ 0.1667 & 0.07492 & 0.9832 \end{pmatrix}$$

and the transformation strain by

$$T_{KS1} = R[5.2644^\circ, [111]]R[9.7356^\circ, [\bar{1}10]]B_3 \simeq \begin{pmatrix} 1.1044 & -0.0728 & 0.1323 \\ 0.0595 & 1.1177 & 0.0595 \\ -0.1917 & -0.0728 & 0.7803 \end{pmatrix}.$$

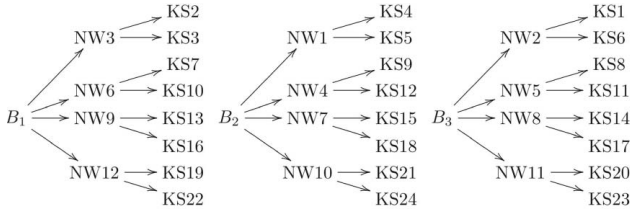
The remaining KS strain variants are  $T_{KSj} := P_jT_{KS1}P_j^T$  and by (14) they are given by

$$T_{KSj} = R[\theta(r), P_j[111]]R[\phi(r), P_j[\bar{1}10]]P_jB_3P_j^T.$$

In particular,  $T_{KSj}$  leaves the close-packed plane  $P_j\mathbf{n}$  and the close-packed direction  $P_j\mathbf{v}$  within that plane unrotated. The corresponding OR variants are given by  $O_{KSj} = P_jO_{KS1}P_j^T$  and  $O_{KSj}$  maps the f.c.c. normal  $P_j\mathbf{n}$  and f.c.c. direction  $P_j\mathbf{v}$  to the b.c.c./b.c.t. normal  $P_j(0r1)_{\alpha'}$  and the b.c.c./b.c.t. direction  $P_j[11\bar{r}]_{\alpha'}$  (see Table A2 in the supporting information).

### 3.3. The transformation with stretch component B<sub>1</sub>

Let us, for example, consider  $P = P_2$ . Then



**Figure 2**  
An arrow from a Bain variant  $B_k$  to an NW variant  $NW_j$  signifies that  $T_{NW_j} = R[\phi(r), \mathbf{v}_j]B_k$  (cf. Table 1). Respectively, an arrow from an NW variant  $NW_j$  to a KS variant  $KS_i$  signifies that  $T_{KS_i} = R[(-1)^{i+1}\theta(r), \mathbf{n}_i]T_{NW_j}$  (cf. Table 2).

**Table 3**  
The OR matrices corresponding to the NW orientation relationships.

Here,  $[h k l] = [1 + 2^{1/2} + 3^{1/2}, 2^{1/2}, -1 + 2^{1/2} + 3^{1/2}] \simeq (0.85, 0.29, 0.44)$ .

OR	OR matrix	OR	OR matrix
NW1	$R[95.264^\circ, [h k l]]$	NW7	$R[95.264^\circ, [\bar{l} \bar{k} h]]$
NW2	$R[95.264^\circ, [l h k]]$	NW8	$R[95.264^\circ, [h \bar{l} k]]$
NW3	$R[95.264^\circ, [k l h]]$	NW9	$R[95.264^\circ, [k \bar{h} l]]$
NW4	$R[95.264^\circ, [\bar{l} k h]]$	NW10	$R[95.264^\circ, [l k \bar{h}]]$
NW5	$R[95.264^\circ, [\bar{h} l k]]$	NW11	$R[95.264^\circ, [h l \bar{k}]]$
NW6	$R[95.264^\circ, [\bar{k} h l]]$	NW12	$R[95.264^\circ, [k h \bar{l}]]$

$$P_2 \mathbf{n} = -\mathbf{n}, P_2 \mathbf{v} = \mathbf{v} \text{ and } P_2 B_3 P_2^T = B_1$$

and thus  $T_{KS2} = R[-\theta(r), [1 1 1]]R[\phi(r), [\bar{1} 1 0]]B_1$  is the only transformation with stretch component  $B_1$  that leaves the close-packed plane  $(111)_\gamma$  and the close-packed direction  $[1 0 \bar{1}]_\gamma$  unrotated. It is therefore the third and last solution of (4).

Just like in the derivation of the NW variants, care has been taken so that all odd  $KS(2j - 1)$  variants correspond immediately to the entries in Table 2 and the crystallographic equivalence in the b.c.c./b.c.t. lattice is given by  $P_{2j-1}^T$ . However, unlike the NW variants,  $T_{KS2} = P_2 T_{KS1} P_2^T \neq T_{KS1}$  are distinct and thus the ORs are different. To illustrate this, let us take  $O_{KS2} = P_2 O_{KS1} P_2^T$  and investigate its action on the f.c.c. plane with normal  $\mathbf{n} = (111)_\gamma$  and the f.c.c. direction  $\mathbf{v} = [1 0 \bar{1}]_\gamma$ . We have

$$O_{KS2} \mathbf{n} = P_2 O_{KS1} (-\mathbf{n}) = -P_2 (0 r 1)_{\alpha'} = (1 r 0)_{\alpha'} \text{ and}$$

$$O_{KS2} \mathbf{v} = P_2 O_{KS1} \mathbf{v} = P_2 [1 1 \bar{r}]_{\alpha'} = [r \bar{1} \bar{1}]_{\alpha'},$$

which are the closest-packed plane and close-packed direction in that plane in the resulting b.c.t. lattice. If  $r = 1$  (b.c.c.), noting that  $P_3 (1 r 0)_{\alpha'} = (0 1 r)_{\alpha'}$  and  $P_3 [r \bar{1} \bar{1}]_{\alpha'} = [\bar{1} r \bar{1}]_{\alpha'}$  we obtain, up to crystallographic equivalence in the b.c.c. lattice (by  $P_3$ ),<sup>5</sup> the OR associated with  $KS2$  (cf. Table 2). The ORs for the remaining even  $KS(2j)$  are obtained analogously and the required crystallographic equivalence transformation in the b.c.c. lattice is given by  $P_3 P_{2j}^T$ . Fig. 2 shows the relations between all Bain, NW and KS variants.

<sup>5</sup> Nevertheless,  $P_3$  is not a lattice-invariant rotation for the resulting b.c.t. lattice.

**Table 4**  
The OR matrices corresponding to the KS orientation relationships.

OR	OR matrix	OR	OR matrix
KS1	$R[+90^\circ, [\bar{1} 2 \bar{1}]]$	KS13	$R[+90^\circ, [\bar{1} 2 \bar{1}]]$
KS2	$R[-90^\circ, [\bar{1} 2 \bar{1}]]$	KS14	$R[-90^\circ, [\bar{1} 2 \bar{1}]]$
KS3	$R[+90^\circ, [\bar{1} \bar{1} 2]]$	KS15	$R[+90^\circ, [\bar{1} 1 2]]$
KS4	$R[-90^\circ, [\bar{1} \bar{1} 2]]$	KS16	$R[-90^\circ, [\bar{1} 1 2]]$
KS5	$R[+90^\circ, [2 \bar{1} \bar{1}]]$	KS17	$R[+90^\circ, [2 1 \bar{1}]]$
KS6	$R[-90^\circ, [2 \bar{1} \bar{1}]]$	KS18	$R[-90^\circ, [2 1 \bar{1}]]$
KS7	$R[+90^\circ, [1 2 \bar{1}]]$	KS19	$R[+90^\circ, [\bar{1} 2 1]]$
KS8	$R[-90^\circ, [1 2 \bar{1}]]$	KS20	$R[-90^\circ, [\bar{1} 2 1]]$
KS9	$R[+90^\circ, [1 \bar{1} 2]]$	KS21	$R[+90^\circ, [\bar{1} \bar{1} 2]]$
KS10	$R[-90^\circ, [1 \bar{1} 2]]$	KS22	$R[-90^\circ, [\bar{1} \bar{1} 2]]$
KS11	$R[+90^\circ, [2 \bar{1} \bar{1}]]$	KS23	$R[+90^\circ, [2 \bar{1} 1]]$
KS12	$R[-90^\circ, [2 \bar{1} \bar{1}]]$	KS24	$R[-90^\circ, [2 \bar{1} 1]]$

### 3.4. Relation to other descriptions

In the literature (see e.g. Kallend *et al.*, 1976; Ray & Jonas, 1990; Bunge, 1982) the NW ORs are sometimes described as  $\zeta = \arccos(1/6^{1/2} - 1/2) \simeq 95.264^\circ$  rotations about  $\langle hkl \rangle$  where  $[h k l] = [1 + 2^{1/2} + 3^{1/2}, 2^{1/2}, -1 + 2^{1/2} + 3^{1/2}]$  and the KS ORs as  $90^\circ$  rotations about  $\langle 112 \rangle$ . We show that these descriptions follow, up to crystallographic equivalence, from the above derivation. Let us start with the OR for NW1. With the choice  $P_3 = R[120^\circ, [1 1 1]]$  we obtain

$$P_3 O_{NW1} = R[\zeta, [h k l]] \simeq R[95.264^\circ, (0.85, 0.29, 0.44)]$$

and thus  $P_{2j-1} P_3 O_{NW1} P_{2j-1}^T = P O_{NWj} = R[\zeta, P_{2j-1} [h k l]]$  for some<sup>6</sup>  $P \in \mathcal{P}^{24}$ . That is, up to crystallographic equivalence in the b.c.c. lattice,  $O_{NWj}$  is a  $\zeta \simeq 95.264^\circ$  rotation about  $P_{2j-1} [h k l]$  (see Table 3).

Next, let us consider the OR for  $KS1$ . With the choice  $P_{10} = R[-120^\circ, [1 \bar{1} 1]]$  we obtain

$$P_{10} O_{KS1} = R[90^\circ, [\bar{1} 2 \bar{1}]]$$

and thus  $P_j P_{10} O_{KS1} P_j^T = P O_{KSj} = R[90^\circ, P_j [\bar{1} 2 \bar{1}]]$  for some<sup>7</sup>  $P \in \mathcal{P}^{24}$ , i.e. up to crystallographic equivalence in the b.c.c. lattice,  $O_{KSj}$  is a  $90^\circ$  rotation about  $P_j [\bar{1} 2 \bar{1}]$  (see Table 4).

### 3.5. Twin relationships between KS variants

With the knowledge of the transformation strains we are able to unambiguously identify pairs of KS variants  $KS_k$  and  $KS_l$  that are twin related, i.e. variant pairs whose relative deformation is an invariant plane strain. That is

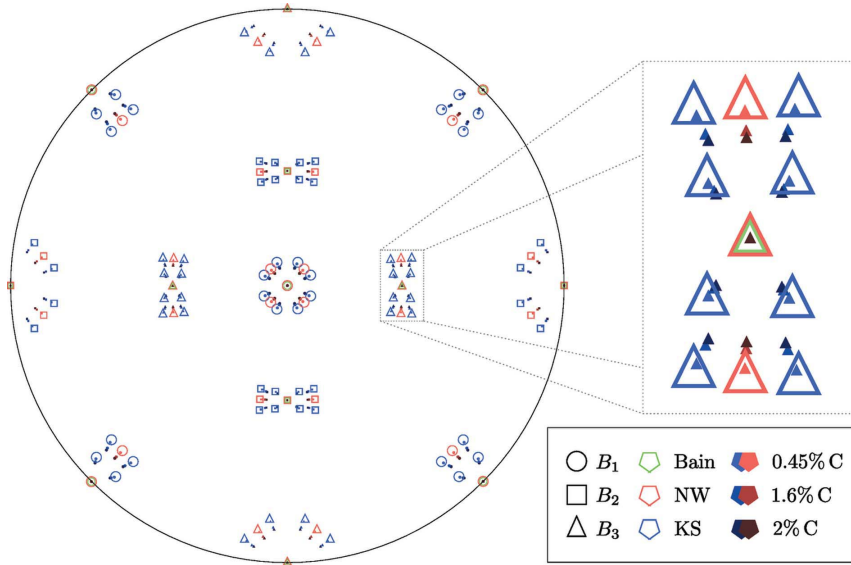
$$T_{KS_k} = T_{KS_l} (\mathbb{I} + \mathbf{b} \otimes \mathbf{m}),$$

where  $\mathbf{b} \otimes \mathbf{m}$  is the  $3 \times 3$  matrix with components  $(\mathbf{b} \otimes \mathbf{m})_{ij} = b_i m_j$ . In particular, this implies that a fully coherent interface of normal  $\mathbf{m}$  can be formed between the two phases. We show that this can only happen between the pairs  $KS(2j - 1)$  and  $KS(2j)$  and whenever this is the case the lattices on either side of the interface are related by a  $180^\circ$  rotation about the common invariant f.c.c. direction

<sup>6</sup>  $P = P_3$  for  $j \in \{1, 2, 3\}$ ,  $P = P_{18}$  for  $j \in \{4, 5, 6\}$ ,  $P = P_{24}$  for  $j \in \{7, 8, 9\}$  and  $P = P_{12}$  for  $j \in \{10, 11, 12\}$ .

<sup>7</sup>  $P = P_j P_{10} P_j^T$ .





**Figure 3** {100} pole figures showing the change in the ORs with increasing carbon content. Hollow circles, squares and triangles correspond, respectively, to the f.c.c. to b.c.c. transformations with stretch components  $B_1$ ,  $B_2$  and  $B_3$ . The colours blue, red and green correspond, respectively, to KS, NW and Bain. The solid shapes correspond to increasing carbon content from lighter to darker shading and with values 0.45, 1.6 and 2 wt% C.

$P_{2j-1}[1\ 0\ \bar{1}] = \mathbf{v}_j$  (cf. Table 1). We start with KS1 and assume that

$$M_i := T_{KS_i} - T_{KS1} = P_i T_{KS1} P_i^T - T_{KS1} = \mathbf{b} \otimes \mathbf{m}. \quad (17)$$

Whenever  $P_i$  does not leave  $\mathbf{v}_1$  invariant we have  $(T_{KS_i} - T_{KS1})\mathbf{v}_1 \neq 0$  and  $(T_{KS_i} - T_{KS1})P_i\mathbf{v}_1 \neq 0$  and thus  $\mathbf{m} \parallel \mathbf{v}_1 \times P_i\mathbf{v}_1$ . Similarly, whenever  $P_i$  does not leave  $\mathbf{n}_1 = (1\ 1\ 1)_\gamma$  invariant, i.e.  $i \geq 7$ , we have<sup>8</sup>  $M_i^T \mathbf{n}_1 \neq 0$  and  $M_i^T \mathbf{n}_i \neq 0$  and thus  $\mathbf{b} \parallel \mathbf{n}_1 \times \mathbf{n}_i$ , where  $\mathbf{n}_i := P_i \mathbf{n}_1$ . Hence, for  $i \geq 7$  it holds that

$$M_i^T \mathbf{n}_i \propto \mathbf{m} \otimes (\mathbf{n}_1 \times \mathbf{n}_i) \mathbf{n}_i = ((\mathbf{n}_1 \times \mathbf{n}_i) \cdot \mathbf{n}_i) \mathbf{m} = 0$$

and thus, since  $\mathbf{n}_i$  is an eigenvector of  $T_{KS_i}^T$ , it must also be an eigenvector of  $T_{KS1}^T$ . However, we know that this can only be the case for  $i \leq 6$  (cf. Table 2), a contradiction. For the remaining cases, i.e.  $2 \leq i \leq 6$ , we have

$$M_i P_i \mathbf{v}_1 \propto \mathbf{b} (\mathbf{v}_1 \times P_i \mathbf{v}_1 \cdot P_i \mathbf{v}_1) = 0$$

and thus since  $P_i \mathbf{v}_1$  is an eigenvector of  $T_{KS_i}$  it must also be an eigenvector of  $T_{KS1}$  which is again, unless  $i = 2$ , a contradiction. Finally,

$$T_{KS2} - T_{KS1} = P_2 T_{KS1} P_2^T - T_{KS1} = \frac{2^{1/6}}{3^{1/2}} \mathbf{v}_1 \otimes [1\ 0\ 1],$$

where  $P_2$  is a 180° rotation about the common f.c.c. direction  $\mathbf{v}_1$ . Through conjugation with  $P_{2j-1}$  we obtain that the relative deformations between  $T_{KS_{2j-1}}$  and  $T_{KS_{2j}} = P_{2j-1} T_{KS2} P_{2j-1}^T$  are also invariant plane strains.

<sup>8</sup> For an invertible matrix  $A$ ,  $\mathbf{v}$  is an eigenvector of  $\text{cof } A$  iff it is an eigenvector of  $A^T$ .

### 3.6. The influence of tetragonality on the orientation relationships

For many compositions of steel the  $\alpha'$  phase is not cubic ( $r = 1$ ) but slightly tetragonal ( $r > 1$ ). For instance, the addition of carbon leads to a ratio of tetragonality approximately given by

$$r = \frac{c}{a} = 1 + 0.045 \text{ wt\% C} \quad (18)$$

for C in the range 0.4–2 wt% C (see Roberts, 1953; Winchell & Cohen, 1962).<sup>9</sup> Similarly, the addition of nitrogen instead of carbon leads to a tetragonality ratio of

$$r = \frac{c}{a} = 0.995 + 0.0383 \text{ wt\% N}$$

for N in the range 0.6–2.9 wt% N [after Nishiyama (1978), Fig. 2.2]. For small carbon content and certain Fe–Ni alloys, such as the Fe–30% Ni alloy investigated in Nishiyama (1934) and Wassermann (1935), the  $\alpha'$  phase is likely to be cubic; however, alloying additional elements such as Cr, Mn or Ti leads

again to a tetragonal  $\alpha'$  phase.

Our derivation in §3 takes the tetragonality of the  $\alpha'$  phase into account and the transformation strains, as well as the ORs, are derived for any ratio of tetragonality  $1 \leq r < 2^{1/2}$ .<sup>10</sup> In particular, the angles of rotations  $\phi(r)$  and  $\theta(r)$  in (9) and (13), respectively, decrease with increasing tetragonality and thus our theory predicts a narrower distribution of peaks in the pole figures. This prediction agrees very well with the work of Ray & Jonas (1990) who summarize that ‘investigators have shown that the chemical composition of steel has a significant effect on the nature and sharpness of the final transformation texture’ and that increasing alloy content (i.e. higher tetragonality) leads to sharper textures [see e.g. Ray & Jonas (1990), Figs. 11–16]. Fig. 3 depicts the changes in the NW and KS ORs for different ratios of tetragonality obtained through (18) for a carbon content increasing from 0% to 2%.

## 4. Other orientation relationship models

In this section, we briefly comment on how our approach can be used to derive the P (see Pitsch, 1959), GT (see Greninger & Troiano, 1949) and GT' (see He *et al.*, 2006) OR models.

### 4.1. The Pitsch model

Following Pitsch (1959) the P ORs are given as<sup>11</sup>

<sup>9</sup> Related experiments on Fe–7% Al–C in Watanabe & Wayman (1971) showed that the tetragonality does not increase for carbon above 2%.

<sup>10</sup> Note that  $r = 2^{1/2}$  corresponds to an f.c.c. lattice and thus there is no phase transformation.

<sup>11</sup> In Pitsch (1959) a third parallelism  $[1\ \bar{1}\ 0]_\gamma \parallel [\bar{1}\ \bar{1}\ 1]_\alpha$  is provided, which is not required for our derivation but, nevertheless, follows from it.

$$(110)_\gamma \parallel (\bar{1}\bar{1}\bar{2})_{\alpha'} \text{ and } [001]_\gamma \parallel [1\bar{1}0]_{\alpha'}. \quad (19)$$

Using our unified approach from §2 with  $\mathbf{n} = (110)$  and  $\mathbf{v} = [1\bar{1}0]$  we obtain  $T_{P1} = R[-\psi(r), [001]]B_2$  and  $O_{P1} = R[-45^\circ, \mathbf{e}_2]R[\psi(r), [001]]$ , where  $\psi(r) = \arccos[(2^{1/2} + r)/(2^{1/2}(2 + r^2)^{1/2})]$ . The remaining 11 P OR and strain variants are given through conjugation with  $\mathcal{P}^{24}$ . We note that for  $r = 1$ ,  $\psi(1) = \phi(1)$ , where  $\phi(r)$  is given by (9) in the derivation of the NW variants, and that  $O_{P1} = O_{NW7}^T$  (similarly  $O_{Pj} = O_{NW_i}^T$  for some  $i$ ). If instead of (19) one uses the parallelisms  $(010)_\gamma \parallel (101)_{\alpha'}$  and  $[101]_\gamma \parallel [\bar{1}11]_{\alpha'}$  (as e.g. in He *et al.*, 2006; Nolze, 2004) the resulting strains and ORs are the same. Finally, we remark that occasionally Pitsch (1962) is also cited for the Pitsch ORs. However, the measurements in Pitsch (1962) are for cementite, which has an orthorhombic crystal structure, and thus our unified approach from §2 does not apply directly. Nevertheless, the underlying mechanism remains applicable if in (4) one replaces the Bain strain by the respective strain required to transform austenite to cementite.

#### 4.2. The Greninger–Troiano and inverse Greninger–Troiano models

Greninger & Troiano (1949) studied an Fe–20%Ni–0.8%C crystal with  $r = c/a = 1.045$  and observed the following approximate parallelisms:

$$(111)_\gamma : (101)_{\alpha'} \simeq 1^\circ, \quad \langle 112 \rangle_\gamma : [10\bar{1}]_{\alpha'} \simeq 2^\circ \\ \text{and } \langle 110 \rangle_\gamma : [1\bar{1}\bar{1}]_{\alpha'} \simeq 2.5^\circ.$$

Apart from these original ORs (up to crystallographic equivalence), several authors use slightly different approximate parallelisms as defining features of the GT ORs. For instance, Bhadeshia & Honeycombe (2006) and Tsai *et al.* (2002) report  $\{111\}_\gamma : \{011\}_{\alpha'} \simeq 0.2^\circ$  and  $\langle 10\bar{1} \rangle_\gamma : \langle 11\bar{1} \rangle_{\alpha'} \simeq 2.7^\circ$ , and He *et al.* (2006) use the parallelisms

$$\{111\}_\gamma \parallel \{011\}_{\alpha'} \text{ and } \langle 51217 \rangle_\gamma \parallel \langle 71717 \rangle_{\alpha'} \quad (20)$$

to approximate the GT ORs. Using the parallelism condition (20) our unified approach can capture the slight misorientations as an effect of the increased tetragonality of the b.c.t. lattice. With  $\mathbf{n} = (111)_\gamma$  and  $\mathbf{v} = [\bar{5}17\bar{1}2]_\gamma$  we obtain  $T_{GT1} = R[\xi(r), [111]]R[\phi(r), [\bar{1}10]]B_3$  and

$$O_{GT1} = R[45^\circ, \mathbf{e}_3]R[-\phi(r), [\bar{1}10]]R[-\xi(r), [111]]$$

with

$$\xi(r) = \arccos\left(\frac{7^2 + 17^2 3^{1/2}(1 + r^2)^{1/2}}{2^{1/2}(5^2 + 12^2 + 17^2)^{1/2}(7^2 + 17^2 + 17^2 r^2)^{1/2}}\right).$$

In particular, we have  $(111)_\gamma \parallel (0r1)_{\alpha'}$  and  $[\bar{1}2\bar{5}17]_\gamma \parallel [\bar{7}\bar{1}717r]_{\alpha'}$  and thus for the value  $r = 1.045$  studied in Greninger & Troiano (1949) we obtain  $(111)_\gamma \parallel (01.0451)_{\alpha'} : (011)_{\alpha'} \simeq 1.26^\circ$ ,  $[112]_\gamma : [01\bar{1}]_{\alpha'} \simeq 2.8^\circ$  and  $[10\bar{1}]_\gamma : [1\bar{1}\bar{1}]_{\alpha'} \simeq 2.9^\circ$ .

The inverse GT introduced in He *et al.* (2006) satisfies the conditions  $(\bar{1}7\bar{7}17)_\gamma \parallel (\bar{5}\bar{1}217)_{\alpha'}$  and  $[101]_\gamma \parallel [111]_{\alpha'}$ , and as

before our unified approach can be used to derive the corresponding strains and ORs. For further details on the P, GT, GT' and also on the NW and KS ORs we refer the reader to the supporting information.

## 5. Conclusions

A unified approach to derive transformation strains and orientation relationship models in steels is presented. An important aspect is the identification of strains with orientation relationships. The unified approach is used to derive the NW, KS and other models and extend them naturally to the situation of a tetragonal  $\alpha'$  phase. The obtained dependence on the ratio of tetragonality seems to be in good qualitative agreement with experiments.

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