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On the relation between orientation relationships predicted by the phenomenological theory and internal twins in plate martensite

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The phenomenological theory of martensite crystallography predicts two equivalent solutions for a particular habit plane in the case of a Fe–Ni–C alloy. Those two solutions differ in the magnitude of the inhomogeneous shear and in the orientation relationship (OR) they hold with austenite. Only the OR associated to the low shear solution has been observed experimentally so far. In the present study, the orientation relationship associated to the high shear solution is assessed experimentally using TEM measurements.

Keywords: Martensite; Crystallography; Twinning; ACOM TEM; Orientation relationship

The major characteristic feature of the substructure of lens martensite forming in high carbon steels or in Fe-High Ni alloys is its internal twinning [1–3]. The amount of internal twinning is known to depend on the transformation temperature in Fe-High Ni alloys [4,5]. In martensite forming at relatively high temperatures, internal twinning is confined in a narrow band known as the midrib. In martensite forming at the lowest temperatures (below about −120 °C in Fe–Ni–C alloys [5]), internal twins extend over the entire thickness of the plate. The presence of such internal defects has commonly been related in the literature to the lattice invariant shear (LIS) hypothesized in the phenomenological theory of martensite crystallography (PTMC) to convert the Bain strain into an invariant plane strain [6]. More precisely, if the LIS system is chosen to be $(1\,0\,1)_\gamma[1\,0\,\bar{1}]_\gamma$, the theory predicts two equivalent possibilities for each habit plane solution. Those two possibilities come from two distinct Bain distortions (whose compressions axis are mirrors of each other through the plane of the LIS) and differ in the magnitude of the LIS. They are referred to as the low and high shear solutions [6,7]. Those two equivalent transformation paths could in principle be distinguished through the orientation relationship they hold with the austenite [8]. In this framework, an internally twinned martensite plate is seen as an alternate stacking of those two orientations referred to as the matrix (low shear solution) and the twin (high shear solution). Those two solutions are formally equivalent and could in principle be formed experimentally. Interestingly, the low shear solution is always produced in preference to the high shear one. Bowles and Mackenzie consequently supposed that the twin orientation was less favoured because of the larger magnitude of the LIS involved in its formation [7]. This preponderance of the low shear orientation may also explain why a single orientation relationship has systematically been reported for lens martensite forming in Fe-High Ni alloys [6,9]. This experimental OR is indeed quite close to the OR predicted by the theory in the low shear case and is located between the Nishiyama–Wassermann (N–W) OR $(\{1\,1\,1\}_\gamma||\{0\,1\,1\}_\alpha, \langle\overline{1\,1}\,2\rangle_\gamma||\langle 0\,\bar{1}\,1\rangle_\alpha)$ and the Kurdjumov–Sachs (KS) OR $(\{1\,1\,1\}_\gamma||\{0\,1\,1\}_\alpha, \langle\bar{1}\,0\,1\rangle_\gamma||\langle\overline{1\,1}\,1\rangle_\alpha)$ [7]. More recent EBSD studies by Shibata et al. have revealed an orientation spread inside lenticular martensite in Fe-High Ni alloys [10,11]. The densely twinned midrib region holds an orientation relationship close to the Greninger–Troiano (GT) OR $(\{1\,1\,1\}_\gamma$ 1° from $\{0\,1\,1\}_\alpha, \langle\bar{1}\,0\,1\rangle_\gamma$ 2.5° from $\langle\overline{1\,1}\,1\rangle_\alpha)$ while the untwined region close to the austenite/martensite interface holds a near K–S OR. Though measurable, the orientation spread measured in lens martensite is small and continuous (about 3°). Furthermore, it was not possible for those authors to index the twin orientation near the midrib. As a consequence, it was not possible for them to measure directly the OR between the twin orientation and the austenite. This may be attributed to the large interaction volume of the SEM-based diffraction techniques (a few 1000 nm^3 at usual acceleration voltages i.e. 15–20 kV) that encompass both the twin and its matrix orientations. Since the volume fraction of the twin orientation is smaller, the resulting Kikuchi pattern is representative of the matrix orientation only. TEM-based diffraction techniques seem therefore more appropriate to study the OR of lens martensite. In a recent TEM analysis of lens martensite, Stormwinter et al. were indeed able to index separately the

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twin and matrix orientations of a martensite plate formed in Fe–1.2C by means of automated crystal orientation measurements (ACOM) [12]. Unfortunately, since no retained austenite was present in the scanned area, those authors were not able to measure the OR between those two orientations and the parent austenite. Hence, the OR associated with the high shear solution has not been measured experimentally yet.

In what follows, the phenomenological theory of martensite is applied for the case of a Fe–30.5Ni–0.155C alloy following the derivation and notations used in [13,14]. The two ORs predicted by the theory are expressed in terms of parallelism conditions between close-packed planes and directions in both phases. The relevance of those predictions is tested against TEM measurements performed on a twinned martensite plate.

The lattice parameters of Fe–30.5%Ni–0.155C determined by X-ray diffraction are $a_\gamma = 0.3591$ nm and $a_\alpha = 0.2875$ nm for austenite and martensite, respectively. The Bain strain matrix in the standard reference frame of austenite reads:

$$\gamma\boldsymbol{B}\gamma = \begin{bmatrix} 1.1322 & & \\ & 1.1322 & \\ & & 0.8006 \end{bmatrix} \tag{1}$$

The lattice invariant shear (LIS) is assumed to be a simple shear on the $\{112\}_\alpha$ plane in the $\langle 111\rangle_\alpha$ direction in martensite. For the present example, the specific variant $(112)_\alpha[11\bar{1}]_\alpha$ is selected and the following variant of the correspondence matrix is chosen:

$$\boldsymbol{\alpha}\boldsymbol{C}\gamma = \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2}$$

By making use of this correspondence matrix, the present variant of the shear system can be expressed in the reference frame of austenite as $(101)_\gamma[10\bar{1}]_\gamma$. The first step in the calculation is to find the line and the plane normal that are left undistorted, though rotated, by the Bain strain. Once defined, those unextended lines and normal will be used to find the rigid body rotation ($\gamma\boldsymbol{R}\gamma$) that allows the Bain strain to be converted into an invariant-line strain ($\gamma\boldsymbol{S}\gamma$). If the undistorted line is chosen to be a normalized vector, lying in the $(101)_\gamma$ plane, which is undistorted by the Bain strain, then its components have to satisfy three equations describing the fact that it lies respectively on a unit sphere, a plane and an ellipsoid [13,14]. When solved simultaneously, those three equations give two solutions for the undistorted line:

$$\boldsymbol{u} = [0.6632\ 0.3467\ \overline{0.6632}]_\gamma,\ \ \boldsymbol{v} = [\overline{0.6632}\ 0.3467\ 0.6632]_\gamma \tag{3}$$

In the same manner, if the undistorted normal is chosen to be a normalized vector, defining a plane containing the $[10\bar{1}]_\gamma$ direction, which is undistorted by the Bain strain, then its components have to satisfy three equations. When solved simultaneously, those three equations give two solutions for the undistorted normal:

$$\boldsymbol{h} = [0.5310\ 0.6603\ 0.5310]_\gamma,\ \ \boldsymbol{k} = [0.5310\ \overline{0.6603}\ 0.5310]_\gamma \tag{4}$$

We have now to find the rigid body rotation which brings the undistorted line and the undistorted normal back to their original positions so as to make them an invariant line and an invariant normal, respectively. However, we have found that there are two undistorted lines and two undistorted normals. There are consequently four ways of choosing pairs of undistorted lines and undistorted normals. We will see that two distinct ORs arise depending on the chosen pair. If $\boldsymbol{u}$ and $\boldsymbol{h}$ are chosen, the rigid body rotation is calculated to be:

$$\gamma\boldsymbol{R}_1\gamma = \begin{bmatrix} 0.9911 & -0.0327 & 0.1285 \\ 0.0187 & 0.9939 & 0.1083 \\ -0.1312 & -0.1050 & 0.9857 \end{bmatrix} \tag{5}$$

which is a rotation of 9.8° about $[0.0537\ \overline{0.0654}\ \overline{0.0129}]_\gamma$. The same calculation can be done using $\boldsymbol{u}$ and $\boldsymbol{k}$ and this gives:

$$\gamma\boldsymbol{R}_2\gamma = \begin{bmatrix} 0.9731 & 0.1050 & 0.2048 \\ -0.0959 & 0.9939 & -0.0537 \\ -0.2092 & 0.0327 & 0.9773 \end{bmatrix} \tag{6}$$

which is a rotation of 13.54° about $[0.0219\ \overline{0.1049}\ \overline{0.0509}]_\gamma$. That is, a distinct rigid body rotation can be obtained with another pair of undistorted lines and undistorted normals. It can be checked that using $\boldsymbol{v}/\boldsymbol{h}$, on the one hand and $\boldsymbol{v}/\boldsymbol{k}$, on the other, leads to rotations that are crystallographically equivalent to those reported for $\boldsymbol{u}/\boldsymbol{k}$ and $\boldsymbol{u}/\boldsymbol{h}$, respectively. Hence, only the solutions involving $\boldsymbol{u}/\boldsymbol{k}$ and $\boldsymbol{u}/\boldsymbol{h}$ will be considered in the following. Then, for the present choice of lattice invariant shear system there exists two different ways for converting the Bain strain into an invariant line strain that read:

$$\gamma\boldsymbol{S}_1\gamma = \gamma\boldsymbol{R}_1\gamma * \gamma\boldsymbol{B}\gamma = \begin{bmatrix} 1.1222 & -0.037 & 0.1029 \\ 0.0212 & 1.1253 & 0.0868 \\ -0.1486 & -0.1188 & 0.7892 \end{bmatrix} \tag{7}$$

$$\gamma\boldsymbol{S}_2\gamma = \gamma\boldsymbol{R}_2\gamma * \gamma\boldsymbol{B}\gamma = \begin{bmatrix} 1.1018 & 0.1189 & 0.1639 \\ -0.1086 & 1.1253 & -0.043 \\ -0.2369 & 0.037 & 0.7824 \end{bmatrix} \tag{8}$$

Hence, using the same variant of the correspondence matrix, there exist two distinct co-ordinate transformation matrices that read:

$$\boldsymbol{\alpha}\boldsymbol{J}_1\gamma = \boldsymbol{\alpha}\boldsymbol{C}\gamma * \gamma\boldsymbol{S}_1\gamma^{-1} = \begin{bmatrix} 0.9042 & -0.8613 & -0.0232 \\ 0.8465 & 0.8944 & -0.2087 \\ 0.1605 & 0.1353 & 1.2313 \end{bmatrix} \tag{9}$$

$$\boldsymbol{\alpha}\boldsymbol{J}_2\gamma = \boldsymbol{\alpha}\boldsymbol{C}\gamma * \gamma\boldsymbol{S}_2\gamma^{-1} = \begin{bmatrix} 0.7668 & -0.9627 & -0.2135 \\ 0.9523 & 0.7932 & -0.1559 \\ 0.2559 & -0.0672 & 1.2208 \end{bmatrix} \tag{10}$$

The following relations between planes and direction can be extracted from $\boldsymbol{\alpha}\boldsymbol{J}_1\gamma$: $(111)_\gamma$ is 0.53° away from $(011)_\alpha$, $[\bar{1}10]_\gamma$ is 1.75° away from $[\bar{1}00]_\alpha$, $[\bar{1}01]_\gamma$ is 3.6° away from $[\bar{1}\bar{1}1]_\alpha$ and $[11\bar{2}]_\gamma$ is 1.67° away from $[01\bar{1}]_\alpha$.