

# QUANTITATIVE EVALUATION OF THE CRYSTALLOGRAPHIC RELATION IN A MARTENSITIC TRANSFORMATION IN AN FE-28%NI ALLOY

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## ABSTRACT

An Fe-28%Ni alloy was annealed for 18 hours at 1080°C and subsequently furnace cooled to room temperature at 1°C/min. As a result of this annealing treatment the parent austenite structure was partially transformed to martensite. The long soaking treatment at 1080°C has produced an austenite structure with an approximate average grain size of 100  $\mu\text{m}$ . This coarse parent structure largely facilitates the investigation of local orientation relations between austenite parent and martensite product grains. The discrete misorientation data were presented in the Rodrigues-Frank space. After appropriate normalization with respect to a random misorientation distribution, it was observed that the Nishiyama-Wasserman reference misorientations (12 variants) show an intensity of 56 random levels, whereas only an intensity of 27 random levels is observed for the Kurdjumov-Sachs reference points. Therefore it is concluded that, in spite of the considerable spread, the N-W correspondence is better obeyed than the K-S relation under the present experimental conditions. The fact that a significant fraction of misorientations is neither close to a N-W nor a K-S coincidence can be attributed to the very high incidence of martensite twins which are present within the product structure.

## 1. INTRODUCTION

In literature, several crystallographic models are provided to describe the  $\gamma$ - $\alpha$  phase transformation for iron. The most important ones are those of Kurdjumov-Sachs, Nishiyama-Wasserman and Bain [1]. These models are based on the correspondence of certain crystallographic planes and directions in the FCC and the BCC lattice, as listed in Table 1.

**Table 1.** Corresponding planes and directions and number of resulting variants for the most important crystallographic transformation models.

	Corresponding Directions	Corresponding Planes	Orientation relation	Number of Variants
Bain	$[110]\gamma // [010]\alpha$	$(001)\gamma // (001)\alpha$	$\langle 1\ 0\ 0 \rangle 45^\circ$	3
K-S	$[101]\gamma // [111]\alpha$	$(111)\gamma // (110)\alpha$	$\langle 1\ 1\ 2 \rangle 90^\circ$	24
N-W	$[211]\gamma // [011]\alpha$	$(111)\gamma // (110)\alpha$	$\langle 3\ 6\ 2 \rangle 95,3^\circ$	12

These crystallographic relations can easily be implemented in more sophisticated phase transformation models [2]. The effective transformation relation, however, is largely dependent on factors such as the chemical composition and mechanical treatment of the material. The determination of the effective relation is usually done by qualitatively comparing the experimentally determined product phase ODF with the modelled counterparts, obtained by applying the various transformation models (cf. Table I) [3]. In this paper, a procedure is described which allows making a quantitative estimate of the validity of a given crystallographic relation. This procedure is entirely based on the processing of orientation microscopy scans, measured on partially transformed structures in an Fe-28%Ni alloy. In order to obtain a more appropriate visualisation of the results, a representation in the Rodrigues-Frank space was used.

## 2. CONCEPT

First the ideal misorientations will be considered between an arbitrary parent phase orientation and all of its possible product orientations, according to the various models

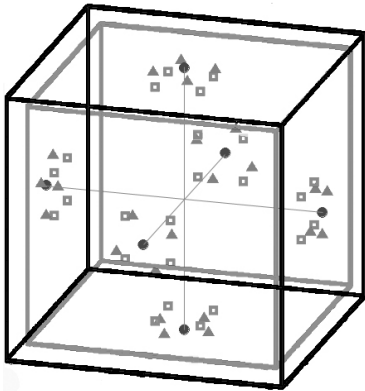


Fig. 1: Representation of the ideal misorientations for the three transformation models Bain (●) N-W (▲) K-S (■)

under investigation (cf. Table I). Depending on the transformation rule under consideration 3, 12 or 24 misorientation variants are associated with the models of Bain, N-W or K-S, respectively. Each of these ideal misorientation variants corresponds to an axis-angle pair  $(d_1, d_2, d_3)\theta$  which can be converted to Rodrigues-Frank coordinates  $(R_1, R_2, R_3)$  by selecting the minimal angle representation  $(d'_1, d'_2, d'_3)\theta_{\min}$  from all cubic symmetric equivalents and applying the following conversion rule on this minimum angle representation [4]:  $(R_1, R_2, R_3) = \tan(\theta_{\min}/2) \cdot (d'_1, d'_2, d'_3)$  with  $(d'_1, d'_2, d'_3)$  being the normalised misorientation axis vector. All calculated misorientations for the three transformation models are represented in Fig. 1.

Since the misorientations, corresponding to the transformation models of Bain and N-W, are positioned on the border of the fundamental zone of the Rodrigues-Frank space

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(outer box), they are also represented by an equivalent point on the opposite face. Therefore Bain and N-W show twice the multiplicity of an arbitrary point, not situated on the edge of the fundamental zone.

These 'ideal' misorientations are compared with the misorientations, obtained from experimental orientation scanning results. Using commercial software [5], each individual grain of a partially transformed structure, can be separated in two partitions, with parent phase gamma and product phase martensite, respectively. The separation should be applied only on these grains in which the parent and product orientations are linked genetically; i.e. when it can be determined with near-certainty that the observed product variants have nucleated from the parent phase in which they are embedded. A representative example of the separation procedure of a single grain is shown in Fig. 2.



Fig.2: The separation of a partially transformed grain into an austenitic (middle) and a martensitic part (right)

Although the parent austenite phase is in principle a single crystal orientation, a considerable spread was observed among the orientation data points of the austenite phase, confined to one single grain. The average parent orientation was determined by superimposing Gaussian distribution peaks on all the austenite data points of a single grain and locating the exact position of the maximum of the ODF thus obtained [6]. In order to determine which product orientations originate from which parent orientations, only the austenitic part of the complete OIM-scan is highlighted, as shown in Fig. 3 (left). This allows defining the former boundaries of the parent grains. The assumption is made that all product grains confined within these boundaries originate from the considered parent grain.

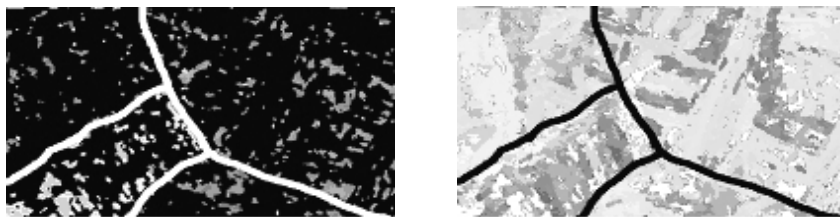


Fig.3: Defining the parent grains, based on the IPF of the gamma phase (left), allows to determine the product orientations for each parent (right).

Subsequently the misorientation between the averaged parent orientation and each pixel of the product phase is calculated and converted to coordinates in the Rodrigues-

Frank space. The position of the experimental misorientation points is compared to the ideal misorientations, corresponding to the various models by determining the fraction of misorientations that are confined within a  $5^\circ$  tolerance from the reference misorientations.

Furthermore, an estimate was made of the volume of these  $5^\circ$  tolerance regions around the ideal reference misorientation. By dividing the above mentioned number fractions by the  $5^\circ$  volume surrounding a given reference point, the number density of the reference point is obtained. These volumes were determined by counting the fractions of misorientations they contained in a random misorientation distribution with  $(3744 \times 3743)/2 = 7006896$  data points. It was established that 1.9% ( $\approx 2\%$ ), 1.0% and 0.25% of these randomly distributed misorientations were positioned within a  $5^\circ$  range from the K-S, N-W and Bain ideal misorientations, respectively. This reflects the respective multiplicities of 1, 2 and 8 for the K-S, N-W and Bain relations.

### 3. EXPERIMENTAL RESULTS AND DISCUSSION

To obtain a partially transformed austenite-martensite structure, an Fe-28%Ni alloy was annealed for 18 hours at  $1080^\circ\text{C}$  and subsequently furnace cooled to room temperature at  $1^\circ\text{C}/\text{min}$  which produced a mixed austenite-martensite microstructure. The long soaking treatment at  $1080^\circ\text{C}$  has produced an austenite structure with an approximate average grain size of  $100\ \mu\text{m}$ .

The above procedure was applied on 3 different areas in the sample. Each OIM-scan consisted of a limited number of grains. In total 9 different grains were examined. The number fractions of misorientations that were observed within  $5^\circ$  of the ideal misorientations are listed in Table 2 for the K-S and N-W relations. The results for the Bain model are not presented since these fractions vary between 0 to 0,25% indicating that the Bain model is not applicable for this material.

**Table 2.** Fractions of the experimental points that are within a  $5^\circ$  distance of the ideal misorientations for N-W and K-S.

	# Pixels	N-W $\pm 5^\circ$	% N-W	KS $\pm 5^\circ$	% K-S
Random	7006869	70904	1.01%	133496	1.91%
Grain 1	10469	7374	70.44%	5731	54.74%
Grain 2	1106	540	48.82%	313	28.30%
Grain 3	47872	38130	79.65%	32044	66.94%
Grain 4	16905	5281	31.24%	5499	32.52%
Grain 5	7966	3164	39.72%	3152	39.57%
Grain 6	18489	5462	29.54%	5275	28.53%
Grain 7	5271	2307	43.77%	3044	57.75%
Grain 8	11861	5877	49.55%	6201	52.28%
Grain 9	7140	3452	48.35%	3669	51.39%
<b>Total</b>	<b>127079</b>	<b>71587</b>	<b>56.33%</b>	<b>64928</b>	<b>51.09%</b>

When the number densities are calculated for the N-W and K-S relations, according to the procedure developed in section 2, it shows that the K-S reference misorientations display an intensity of  $26.9 \times$  random levels whereas for the N-W ideal misorientations an intensity of  $55.7 \times$  random levels is observed. The high intensity of the predicted misorientations can be visualised by plotting all misorientations in the Rodrigues-

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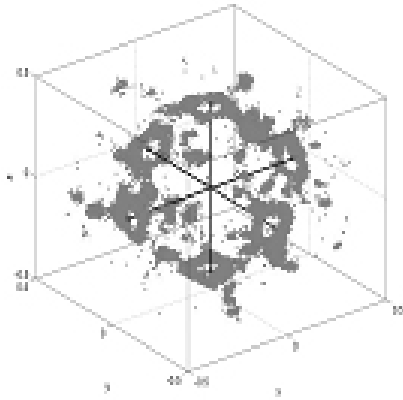


Fig. 4: R-F representation of the measured misorientations for the nine grains

Frank space, as shown in Fig 4. By making the comparison of Fig 4 with Fig 1 it is obvious that most of the misorientation points are located in the vicinity of the N-W and K-S reference misorientations. It is also clear that the Bain model does not give an accurate description of the transformation process, as the R-F volume about the Bain reference points is totally depleted of data.

In spite of these high number densities for the N-W and K-S relations, a considerable fraction of the data points does not correspond to any of the models, mentioned above. Three different reasons can be mentioned to account for the observed deviations. First of all the calculation of

the parent orientation is based on the remaining austenitic phase within the material. The induced stresses during phase transformation unavoidably produce a plastic strain in the remaining austenite, which results in a change of orientation. Small variations on the parent orientations can produce considerable shifts, though, on the number fractions of misorientation data confined to the  $5^\circ$  tolerance volumes around the model reference misorientations. E.g. if the parent orientation of grain 6 is shifted only  $4^\circ$  away from its initial position, it will give rise to an increase of the N-W number fraction from 29% to 54%. A second reason for the large scatter in the observed fractions is twinning which occurs in the product phase, in order to accommodate for the transformation shear strain. This twinning will produce a reorientation in the product phase of  $60^\circ$  about a  $\langle 111 \rangle$ -axis and thus typical twin boundaries will appear in the product phase, cf. Fig 5. This also results in unexpected clusters of points in R-F space as can be observed in Fig 4, since a large area within the product phase is subjected to an identical change in orientation and thus also to an identical change in misorientation with respect to the parent orientation. Finally the observed fractions can also be affected by inaccurate linking of certain product orientations to their assumed parent grain. This is possible if a product grain occurs at the boundary of two former austenitic grains or if martensite laths from upper or underlying parent grains penetrate the two-dimensional observation section. All three reasons can contribute to a decrease of the fraction of misorientations, confined within the considered range near the ideal misorientations. The influence on the ratio, considering the different transformation models, will however be negligible. Therefore, from these results it can be concluded that the Bain model is not at all applicable for this material and that the Nishiyama-Wasserman relation (55 random levels) has a better correspondence with the actual phase transformation in Fe28%Ni than the Kurdjumov-Sachs relation (27 random levels).

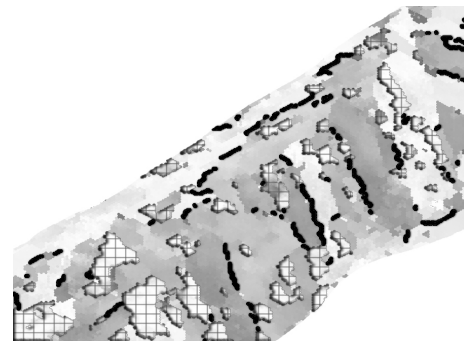


Fig. 5: Highlighting of the  $60^\circ \langle 111 \rangle$  twin boundaries in the alpha phase of grain 4

#### 4. CONCLUSIONS

In order to quantitatively investigate the crystallographic features of a martensitic phase transformation, a partially transformed microstructure was observed. To this purpose, an Fe-28%Ni alloy was annealed for 18 hours at 1080°C and subsequently furnace cooled to room temperature at 1°C/min. By means of orientation microscopy scans the local misorientation carried by the austenite-martensite interface could be measured. All misorientation data between neighbouring parent and the product grains were calculated and expressed in Rodrigues-Frank coordinates. The obtained misorientations were compared with the misorientations corresponding to an ideal transformation, according to the crystallographic relations of Bain, K-S and N-W, allowing a 5° tolerance from these perfect relations. The processed data showed that the N-W relation occurs with a number frequency of 56 random levels, whereas the K-S relations only show an intensity of 27 random levels (allowing for a misfit of max. 5° with respect to these ideal references). The Bain relation was not observed at all. The number intensities of these perfect misorientations vary considerably between individual grains. This was attributed to the experimental spread in the parent grain and to the occurrence of deformation twins in the martensite laths.

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