Short Communication

Orientation relationships between adjacent plates of acicular ferrite in steel weld deposits

The results of an investigation of the orientation relationships between adjacent plates of acicular ferrite are reported in an attempt to elucidate further the mechanism of acicular ferrite formation. Welds were made using the manual metal arc technique and the as deposited microstructure of the high strength steel weld deposits was examined using crystallography and transmission electron microscopy. It was found that clusters of acicular ferrite form in such a way that adjacent plates tend to have a similar orientation in space; the reasons for this are discussed.
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©1989 The Institute of Metals. Manuscript received 28 March 1988; in final form 25 July 1988. At the time the work was carrtied out the authors were in the Department of Materials Science and Metallurgy, University of Cambridge. Professor Yang is now at the Taiwan National University, Taipei, Taiwan.

Introduction

Acicular ferrite is just one component of the complex microstructure that develops in steel weld deposits. It is useful to begin with a brief consideration of acicular ferrite in the context of weld metal tranformation products. Detailed discussions of the transformation mechanisms and other features of weld microstructures can be found in some recent reviews.[1–4]

Allotriomorphic ferrite (α) is the first phase to form during the cooling of austenite in low alloy steel welds. It nucleates at the austenite grain boundaries and grows by a diffusional transformation mechanism. The growth of allotriomorphic ferrite is anisotropic, the rate being highest along the austenite grain boundaries, which soon become decorated by layers of α.

As the transformation temperature decreases, processes involving diffusion become sluggish and *displacive* transformations are then kinetically (though not thermodynamically) favoured. Displacive transformations do not involve any reconstructive diffusion,[4] the substitutional alloying additions and the iron atoms being configurationally 'frozen' during reaction. Consequently, the transformations are accompanied by macroscopic displacements reflecting the coordinated movement of atoms during the lattice change, the displacements having the characteristics of invariant-plane strains. Thus, their morphology is dominated by the necessity to minimise strain energy. Plates of Widmanstätten ferrite (α_W) grow at relatively low undercoolings by a displacive, paraequilibrium mechanism which involves the simultaneous growth of pairs of mutually accommodating plates of ferrite, so that the strain energy of transformation is reduced.

On further cooling, acicular ferrite nucleates intragranularly on inclusions in the weld; its presence is associated with an improvement in the toughness of the weld deposit (e.g. *see* Refs. 1–3, 5–9). Acicular ferrite has a thin plate morphology and the transformation is found to exhibit an 'incomplete-reaction phenomenon' in the sense that the formation of acicular ferrite ceases before the residual austenite reaches its equilibrium composition.[10,11] The growth of acicular ferrite is known to be accompanied by an invariant-plane strain shape deformation[11] so that there is an atomic correspondence between the parent and product lattices, at least as far as the atoms in substitutional sites are concerned. Consequently, a plate of acicular ferrite always has its closest packed plane almost parallel to a corresponding close packed plane of the austenite in which it grows, and corresponding close packed directions within these planes are also found to be parallel or almost parallel.[11] Thus, the orientation relationship with the austenite is always within the Bain region and often similar to the classical Kurdjumov–Sachs and Nishiyama–Wasserman orientation relationships.[11] This discussion is of particular significance for weld microstructures, because it is sometimes implied[12] that there is a reproducible orientation relationship between acicular ferrite and the inclusions on which it may nucleate. However, there is no evidence for this.[13] Considering together the facts that the orientation of an inclusion (which forms in the liquid steel) is random in space and that the orientation of the acicular ferrite, by virtue of its displacive transformation mechanism, must be within the Bain region, it follows that the orientation relationship between the inclusion and acicular ferrite must also be random.

Although the plates of acicular ferrite which form first nucleate heterogeneously on the non-metallic inclusions that are common in weld deposits,[2–3, 5–9] it seems that subsequent plates can form 'sympathetically',[14] so that a one-to-one correspondence between inclusions and acicular ferrite plates is not expected. This is reasonable since the shape change associated with the transformation should favour the formation of mutually accommodating variants, as occurs during the autocatalytic effects associated with the well known classical bursts of martensitic transformation.[15,16] If such effects occur during the formation of acicular ferrite, then it is expected that adjacent variants should have different shape deformations (and habit planes), but should tend to be in a similar orientation in space (or be approximately twin related).[17] In another context, it is reported that the boundary between adjacent plates of acicular ferrite can be described as 'high-angle', and Ito *et al.*[18] have stated that the angle between adjacent plates of acicular ferrite is about 26°. However, it is not appropriate to describe either the structure of a boundary or the misorientation between grains in terms of just an angle of rotation (e.g. *see* Refs. 19, 20). The description of an orientation relationship between grains of identical structure itself requires three degrees of freedom: the angle of rotation and two direction cosines representing the axis of rotation. As is shown below, additional ambiguity is introduced by symmetry considerations, since they imply that the misorientation angle is not unique for the crystal structure considered.

Table 1 Results of chemical analysis, wt-%

C	Si	Mn	P	S	Cr	Mo	Ni	Al	N	Nb	Ti	V	O
0·031	0·40	1·68	0·008	0·005	0·04	0·17	2·46	0·02	0·0080	0·01	0·03	0·01	0·0333

In the present work, an investigation of orientation relationships between neighbouring plates of acicular ferrite is reported in an effort to elucidate further the mechanism of its formation.

Method

WELDING PROCEDURE

The weld was made using the manual metal arc technique using 4 mm dia. electrodes (E10016-G type as defined by the American Welding Society), the joint geometry being designed according to BS 639 to avoid dilution from the base plate. The welding was carried out in the flat position using the stringer bead technique, the parent plate thickness being 20 mm. The welding current and voltage used were 180 A and 23 V (dc+) respectively (nominal arc energy ≈2 kJ mm^{-1}), the weld consisting of some 21 runs with 3 runs per layer, deposited at a speed of about 0·002 m s^{-1}; the interpass temperature was typically 250°C.

This weld is a part of a series of high strength weld deposits in which the primary microstructure consists essentially of acicular ferrite together with a small quantity of martensite and retained austenite.[10,21] The specimens studied in the present work were taken from the top layer of the multirun weld deposit and contained just the as deposited microstructure.

ANALYSIS

The chemical analysis (Table 1) was carried out using a spectroscopic technique, although the concentrations of oxygen and nitrogen were measured using Leco furnaces (Ro 17 and Tn 15) with 50 g of material for each determination to ensure representative results.

SAMPLE PREPARATION

Samples for transmission electron microscopy were prepared from 3 mm dia. discs machined from the top layer of the weld, containing the as deposited, primary microstructure. The discs were mechanically ground down to a thickness of 0·08 mm on 1200 grit SiC paper; then the specimens were twin jet electropolished using a 5% perchloric acid, 25% glycerol, and 70% ethanol mixture at ambient temperature and 45 V. They were examined using a Philips EM 400T transmission electron microscope operated at 120 kV.

Table 2 Orientation relationships between adjacent plates of acicular ferrite: axes are referred to crystallographic basis and rotation operations are right handed

Number	Axis angle pair
1	⟨0·131 0·991 0·000⟩ 180°
2	⟨0·139 0·990 0·000⟩ 180°
3	⟨0·113 0·994 0·000⟩ 180°
4	⟨0·131 0·991 0·000⟩ 180°
5	⟨0·743 0·078 0·665⟩ 180°
6	⟨0·743 0·078 0·665⟩ 180°
7	⟨0·734 0·057 0·677⟩ 180°
8	⟨0·729 0·046 0·683⟩ 180°
9	⟨0·785 0·208 0·609⟩ 175°
10	⟨0·729 0·138 0·671⟩ 179°
11	⟨0·717 0·368 0·593⟩ 173°
12	⟨0·639 0·617 0·460⟩ 179°
13	⟨0·797 0·365 0·481⟩ 179°
14	⟨0·859 0·168 0·483⟩ 175°
15	⟨0·885 0·258 0·389⟩ 174°

CRYSTALLOGRAPHIC TECHNIQUES

The orientation relationship between a pair of like crystals, the crystallographic bases of which are defined from a common origin, can be described using an axis angle pair. From this it can be inferred that if one of the crystals is rigidly rotated about the specified axis which passes through the origin, through a right-handed angle of rotation θ, its orientation coincides with that of the other.

Accurate measurements of orientation relationships are best carried out using Kikuchi lines, but this proved difficult in the present work, since the high dislocation density of the acicular ferrite makes the Kikuchi lines rather diffuse. On the other hand, to demonstrate that adjacent plates are approximately in the same orientation in space does not require extreme precision, so the experimental data are based on the analysis of the reciprocal lattice vectors observed in conventional selected area electron diffraction patterns. The zone axis of the pattern can then deviate typically by 5° from the optic axis of the microscope, and this can be used as an estimate of error. In fact, the error should be somewhat lower, since orientations were deduced not from the zone axes, but by examining the relationship between pairs of reciprocal lattice vectors (in the same diffraction pattern) from each of the two crystals concerned. The four reciprocal lattice vectors were used to deduce the rotation matrix, and hence the axis angle pair, in the manner described* elsewhere.[19,20]

Because acicular ferrite has a bcc crystal structure, there are in general 24 crystallographically equivalent descriptions (in terms of axis angle pairs or rotation matrices) of any

Table 3 Crystallographically equivalent axis angle pairs for first row of experimental data in Table 2: axes are referred to crystallographic basis and rotation operations are right handed

⟨0·131 0·991 0·000⟩	180°
⟨0·000 0·000 1·000⟩	15°
⟨0·000 0·000 1·000⟩	75°
⟨0·477 0·622 0·622⟩	129°
⟨0·520 0·678 0·520⟩	112°
⟨0·093 −0·704 0·704⟩	169°
⟨0·793 0·609 0·000⟩	180°
⟨−0·704 −0·093 0·704⟩	169°
⟨0·983 0·129 0·129⟩	91°
⟨−0·129 0·983 −0·129⟩	91°
⟨0·609 0·793 0·000⟩	180°
⟨0·622 −0·477 −0·622⟩	129°
⟨0·678 −0·520 0·520⟩	112°
⟨0·000 0·000 1·000⟩	165°
⟨0·983 0·129 −0·129⟩	91°
⟨0·704 0·093 0·704⟩	169°
⟨0·000 0·000 −1.000⟩	105°
⟨−0·678 0·520 0·520⟩	112°
⟨−0·520 −0·678 0·520⟩	112°
⟨0·129 −0·983 −0·129⟩	91°
⟨−0·093 0·704 0·704⟩	169°
⟨0·477 0·622 −0·622⟩	129°
⟨−0·622 0·477 −0·622⟩	129°
⟨0·991 0·131 0·000⟩	180°

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* The procedure for doing such calculations is illustrated with worked examples in Ref. 20; examples 4–6 are particularly relevant. A computer program capable of carrying out these calculations, on any IBM PC compatible computer using an MS DOS operating system can be obtained by contacting the present authors.

orientation relationship. The equivalent operations can be generated by multiplying the rotation matrix by the symmetry operations of the bcc structure. Hence, for each experimentally determined orientation relationship, all 24 possibilities were calculated; following convention, that with the highest angle of rotation was chosen for presentation in Table 2.

Analysis of the data revealed that in two cases, the axis angle pairs were close to ⟨1 1 1⟩ about 180°. These data are ambiguous, since it can be deduced either that the plates are in the same orientation in space or that they are related by a $\Sigma 3$ orientation. (The term Σ refers to coincidence site lattice theory[12,13,22,23] and represents the reciprocal density of coincidence sites found when the two lattices with a common origin are allowed to interpenetrate notionally and fill all space.) Owing to the ambiguity of interpretation, these two sets of data are not included in the discussion that follows.

Plates of acicular ferrite can appear to be adjacent to one another for two different reasons: the formation of one plate may stimulate the growth of another or plates which have nucleated at completely separate sites may come in contact as a consequence of impingement. Care was taken to examine only the former case; at low magnifications, sympathetically nucleated plates can be seen to grow in clusters.

Results and discussion

The results from several experiments are presented in Table 2. The components of the axes concerned are rounded-off to three decimal places; this level of accuracy may not be justified by the experimental technique, but any further rounding-off in some cases can give a misleading impression of the rationality of the axis of rotation. The angles are rounded-off to integers. To illustrate the effect of symmetry, the 24 crystallographically equivalent axis angle pair representations of the first row of the results presented in Table 2 are listed in Table 3; obviously, it is not appropriate to state the orientation in terms of a unique angle of misorientation.

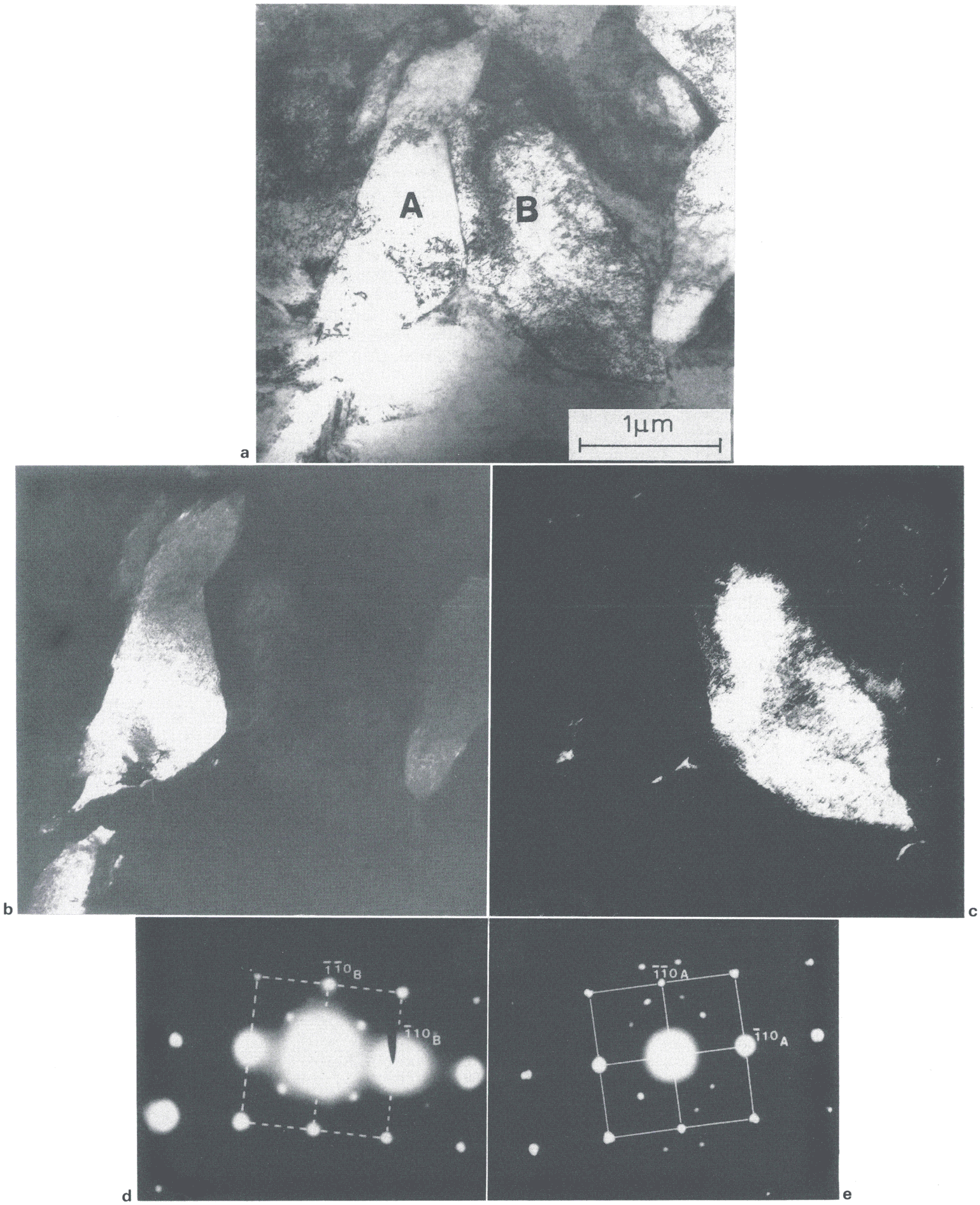
It can be seen from the results in Table 2 that most (1–10) of the adjacent plates are similarly orientated in space, the axis angle pairs being close to the symmetry operations 180° about ⟨0 0 1⟩ or 180° about ⟨0 1 1⟩ of the bcc structure. With the exception of no. 11, all the others are close to low Σ orientations. Numbers 12 and 15 are close to a $\Sigma = 11$ orientation (i.e. 180° about ⟨1 1 3⟩), no. 13 is close to $\Sigma = 3$ orientation (i.e. 180° about ⟨1 1 2⟩). Number 14 can also be described by the axis angle pair 34·2° about ⟨0·636 0·767 0·086⟩, which is close to a $\Sigma = 9$ orientation (i.e. 38·9° about ⟨1 1 0⟩).

Table 4 Axis angle pairs (with respect to α) relating variant number 1 to other variants of ferrite that may form within same austenite crystal

	γ orientation	Axis angle pair	Equivalent axis angle pair
Nishiyama–Wasserman α–γ orientation relationship (11 other variants of ferrite)*			
1	$(1\,1\,1)[\bar{1}\,0\,1]$	[1·000 0·000 0·000] 0°	… … … …
2	$(1\,1\,1)[0\,1\,\bar{1}]$	[0·000 −0·707 −0·707] 120°	⟨0·866 0·354 0·354⟩ 180°
3	$(1\,1\,1)[1\,\bar{1}\,0]$	[0·000 0·707 0·707] 120°	⟨0·866 0·354 0·354⟩ 180°
4	$(1\,1\,\bar{1})[\bar{1}\,1\,0]$	[−0·707 −0·697 −0·120] 90°	⟨0·702 0·560 0·440⟩ 179°
5	$(1\,1\,\bar{1})[1\,0\,1]$	[0·000 −0.169 0·986] 90°	⟨0·707 0·697 0·120⟩ 180°
6	$(1\,1\,\bar{1})[0\,\bar{1}\,\bar{1}]$	[0·500 0·373 0·782] 180°	⟨0·782 0·500 0·373⟩ 180°
7	$(1\,\bar{1}\,1)[\bar{1}\,\bar{1}\,0]$	[−0·707 0·697 0·120] 90°	⟨0·702 0·560 0·440⟩ 179°
8	$(1\,\bar{1}\,1)[1\,0\,\bar{1}]$	[0·000 0·986 0·169] 180°	⟨0.986 0.169 0·000⟩ 180°
9	$(1\,\bar{1}\,1)[0\,1\,1]$	[−0·707 −0·697 −0·120] 90°	⟨0·702 0·560 0·440⟩ 179°
10	$(\bar{1}\,1\,1)[\bar{1}\,0\,\bar{1}]$	[0·000 0·169 −0·986] 90°	⟨0·707 0·697 0·120⟩ 180°
11	$(\bar{1}\,1\,1)[1\,1\,0]$	[0·500 0·373 0·782] 180°	⟨0·782 0·500 0·373⟩ 180°
12	$(\bar{1}\,1\,1)[0\,\bar{1}\,1]$	[0·707 0·697 0·120] 90°	⟨0·702 0·560 0·440⟩ 179°
Kurdjumov–Sachs α–γ orientation relationship (23 other variants of ferrite)†			
1a	$(1\,1\,1)[\bar{1}\,0\,1]$	[1·000 0·000 0·000] 0°	… … … …
1b	$(\bar{1}\,\bar{1}\,\bar{1})[\bar{1}\,0\,1]$	[0·577 0·577 0·577] 180°	⟨0·577 0·577 0·577⟩ 180°
2a	$(1\,1\,1)[0\,1\,\bar{1}]$	[0·000 −0·707 −0·707] 120°	⟨0·612 0·612 0·500⟩ 180°
2b	$(\bar{1}\,\bar{1}\,\bar{1})[0\,1\,\bar{1}]$	[0·996 0·065 0·065] 180°	⟨0·996 0·065 0·065⟩ 180°
3a	$(1\,1\,1)[1\,\bar{1}\,0]$	[0·000 0·707 0·707] 120°	⟨0·612 0·612 0·500⟩ 180°
3b	$(\bar{1}\,\bar{1}\,\bar{1})[1\,\bar{1}\,0]$	[0·418 0·642 0·642] 180°	⟨0·418 0·642 0·642⟩ 180°
4a	$(1\,1\,\bar{1})[\bar{1}\,1\,0]$	[−0·742 −0·650 −0·167] 90°	⟨0·696 0·584 0·417⟩ 175°
4b	$(\bar{1}\,\bar{1}\,1)[\bar{1}\,1\,0]$	[0·856 0·043 −0·515] 120°	⟨0·742 0·500 0·446⟩ 176°
5a	$(1\,1\,\bar{1})[1\,0\,1]$	[−0·667 0·742 0·075] 90°	⟨0·705 0·538 0·463⟩ 176°
5b	$(\bar{1}\,\bar{1}\,1)[1\,0\,1]$	[0·075 0·167 0·983] 180°	⟨0·983 0·167 0·075⟩ 180°
6a	$(1\,1\,\bar{1})[0\,\bar{1}\,\bar{1}]$	[0·053 0·984 0·171] 180°	⟨0.984 0·171 0·053⟩ 180°
6b	$(\bar{1}\,\bar{1}\,1)[0\,\bar{1}\,\bar{1}]$	[0·770 −0·149 0·621] 120°	⟨0·734 0·563 0·380⟩ 177°
7a	$(1\,\bar{1}\,1)[\bar{1}\,\bar{1}\,0]$	[0·742 0·650 0·167] 90°	⟨0·696 0·584 0·417⟩ 175°
7b	$(\bar{1}\,1\,\bar{1})[\bar{1}\,\bar{1}\,0]$	[−0·087 −0·900 0·428] 120°	⟨0·862 0·417 0·288⟩ 179°
8a	$(1\,\bar{1}\,1)[1\,0\,\bar{1}]$	[0·471 0·342 0·813] 180°	⟨0·813 0·471 0·342⟩ 180°
8b	$(\bar{1}\,1\,\bar{1})[1\,0\,\bar{1}]$	[0·667 0·742 0·075] 180°	⟨0·742 0·667 0·075⟩ 180°
9a	$(1\,\bar{1}\,1)[0\,1\,1]$	[0·075 0·167 −0·983] 90°	⟨0·992 0·121 0·046⟩ 179°
9b	$(\bar{1}\,1\,\bar{1})[0\,1\,1]$	[−0·856 −0·043 0·515] 120°	⟨0.742 0·500 0·466⟩ 176°
10a	$(\bar{1}\,1\,1)[\bar{1}\,0\,\bar{1}]$	[0·667 −0·742 −0·075] 90°	⟨0·705 0·538 0·463⟩ 176°
10b	$(1\,\bar{1}\,\bar{1})[\bar{1}\,0\,\bar{1}]$	[0·742 0·650 0·167] 180°	⟨0·742 0·650 0·167⟩ 180°
11a	$(\bar{1}\,1\,1)[1\,1\,0]$	[0·524 0·407 0·748] 180°	⟨0·748 0·524 0·407⟩ 180°
11b	$(1\,\bar{1}\,\bar{1})[1\,1\,0]$	(−0·770 0·149 −0·621] 120°	⟨0·734 0·563 0·380⟩ 177°
12a	$(\bar{1}\,1\,1)[0\,\bar{1}\,1]$	[−0·075 −0·167 0·983] 90°	⟨0·992 0·121 0·046⟩ 179°
12b	$(1\,\bar{1}\,\bar{1})[0\,\bar{1}\,1]$	[0·087 0·900 −0·428] 120°	⟨0·862 0·417 0·288⟩ 179°

* When the austenite–ferrite orientation is described by the Nishiyama–Wasserman relationship, the $\{1\,1\,1\}_\gamma$ plane should be taken to be parallel to the $(0\,1\,1)_\alpha$ plane, and the $\langle 1\,0\,\bar{1}\rangle_\gamma$ direction should be taken to be parallel to the $[1\,0\,0]_\alpha$ direction. Note that there are 24 equivalent ways of describing the orientation relationship between any two plates of ferrite, and that giving the highest angle of rotation is also listed under the column heading 'Equivalent axis angle pair'.

† When the austenite–ferrite orientation is described by the Kurdjumov–Sachs relationship, the $\{1\,1\,1\}_\gamma$ plane should be taken to be parallel to the $(0\,1\,1)_\alpha$ plane, and the $\langle 1\,0\,\bar{1}\rangle_\gamma$ direction should be taken to be parallel to the $[\bar{1}\,\bar{1}\,1]_\alpha$ direction. Note that there are 24 equivalent ways of describing the orientation relationship between any two plates of ferrite, and that giving the highest angle of rotation is also listed under the column heading 'Equivalent axis angle pair'. The designations 'a' and 'b' after the identifying numbers refer to pairs of plates which are in $\Sigma = 3$ orientation with respect to each other.



a bright field TEM image of two plates; *b, c* corresponding dark field TEM images of plates A and B, respectively; *d, e* corresponding diffraction patterns of dark field images in *b* and *c*, respectively

1 Set of two typical adjacent plates of acicular ferrite

A typical set of adjacent plates analysed, together with the corresponding diffraction data are shown in Fig. 1; further sets of metallographic results are documented in Ref. 21.

The tendency for adjacent plates of acicular ferrite (α) to form a similar orientation in space could be for two reasons: obviously, during sympathetic nucleation, the formation of plates of approximately the same orientation may be kinetically favoured or the observed tendency may simply be a reflection of the nature of the austenite–ferrite orientation relationship. Hence, calculations were carried out to determine the axis angle pairs relating crystallographic variants of ferrite grains growing within the same austenite (γ) crystal.

The results for the Nishiyama–Wasserman and Kurdjumov–Sachs α–γ orientation relationships are presented in Table 4. Note that there are only 12 variants of the Nishiyama–Wasserman orientation relationship, but 24 of the Kurdjumov–Sachs orientation relationship. This is because, in the latter case, a close packed $\langle 1\,1\,0\rangle_\gamma$ direction is *exactly* parallel to a close packed $\langle 1\,1\,1\rangle_\alpha$ direction. A symmetry operation on the γ lattice, of a rotation of 180° about the $\langle 1\,1\,0\rangle_\gamma$ is equivalent to a *twinning* rotation of 180° about $\langle 1\,1\,1\rangle_\alpha$. Thus, a twin of ferrite is generated while retaining the Kurdjumov–Sachs orientation relationship.

By comparing the data of Table 2 with the results in Table 4, it can be seen that all the experimentally observed axis angle pairs can be explained approximately as resulting from the existence of an α–γ orientation relationship. (Note that only approximate agreement with the calculations is expected, since the actual α–γ orientation relationship is fairly variable.[11]) However, it is evident that in Table 4 only variants 5, 8, and 10 of the Nishiyama–Wasserman relationship give plates which are similarly orientated with respect to variant 1. Similarly, only variants 2b, 5b, 6a, 8b, 9a, and 12a of the Kudjumov–Sachs relationship give plates which are similarly orientated with respect to variant 1. Consequently, if all possible plates form with equal probability, then only a quarter of the plates would be similarly orientated in space. This can be compared with the much higher proportion found experimentally and it can be inferred that adjacent plates of acicular ferrite have a definite tendency to form in a similar orientation in space, perhaps because sympathetic nucleation is then easier.

Conclusions

The orientation relationships that develop between adjacent plates of acicular ferrite in the primary microstructure of a high strength steel weld deposit have been determined. It can be seen from the results that clusters of acicular ferrite plates form in such a way that adjacent plates tend to have a similar orientation in space. This may arise because during sympathetic nucleation, it is easier to form plates with approximately the same orientation.

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