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BCC-BCC ORIENTATION RELATIONSHIPS, SURFACE RELIEF AND DISPLACIVE PHASE TRANSFORMATIONS IN STEELS

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Introduction

In the FCC→HCP martensite transformation**, a degeneracy exists such that the operation of any one of a set of three Shockley partial dislocations on a given $\{111\}_\gamma$ plane generates the same variant of the HCP martensite. This allows minimization of the overall strain energy since the shape strain can be better accommodated by the successive operation of different Shockley partials (1,2). Ignoring the volume change accompanying the FCC→HCP transformation, the required $\frac{a}{6}<112>_\gamma$ simple shear on successive $\{11\bar{1}\}_\gamma$ planes amounts to the total transformation strain. However, a single invariant-plane strain cannot generate the BCC lattice from an FCC structure; the operation of a combination of lattice deformations is necessary. Hence, for the FCC→BCC transformation it is not obvious whether different sets of transformation strains can result in the formation of BCC variants with identical crystallographic orientation relative to a given austenite orientation. Such a situation could arise if the axis-angle pair relating the martensite variants amounts to a symmetry operation on the martensite lattice.

Any degeneracy in the FCC→BCC transformation could have important implications on the interpretation of surface relief effects, as observed on pre-polished and transformed specimens. For instance, tent-like (or vee-shaped) surface displacements have been observed in association with Widmanstätten ferrite (3,4) and lower bainite (5). These displacements are difficult to understand if they are considered to arise from single plates. While it has been suggested (2) that such displacements could arise from the juxtaposition of two variants of the transformation product, such a possibility can only follow if a degeneracy of the type discussed above exists, since the tent-like relief of Widmanstätten ferrite has been shown (6) to originate from single crystal regions of the BCC phase. A degeneracy would allow the two components of the tent to be in identical crystallographic orientation, and yet have different and evidentally mutually accommodating shape strains.

Considering next the martensite and bainite transformations in low-alloy steels, it is frequently observed that neighbouring laths in the packets of martensite or bainite exhibit the same crystallographic orientation. Clearly, in the absence of any degeneracy, each lath should exhibit the same shape strain as its neighbours. Intuitively, the resulting poor overall accommodation of shape strains would not justify the formation of such packets.

The aim of the present study was to seek any degeneracies associated with the FCC→BCC transformation and to discuss the implications of the findings with respect to current ideas on the mechanisms of phase transformations in steels. Only the FCC→BCC transformation is discussed since low alloy steel martensites generally form well above the Zener ordering temperature, and hence do not exhibit tetragonality. The method involved the calculation of the axis-angle pairs relating each of the 24 independent martensite variants to an adopted

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** The abbreviations FCC, HCP and BCC refer to face centered cubic, hexagonal close packed and body centered cubic lattices respectively.

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standard variant; well established crystallographic methods (7,8) were used for this purpose, and both the Kurdjumov-Sachs (9) and the Nishiyama-Wasserman (10,11) austenite-martensite orientation relationships were tested.

Results and Discussion

The full analysis of all the possible axis-angle pairs is given elsewhere (12), and only the relevant variants are considered below.

It was found that an exact degeneracy is indeed possible when the operative γ/α orientation relationship is that of Nishiyama and Wasserman (NW). In table 1, NW1 represents the adopted standard variant, right-handed rotations are taken to be positive and the rotations are relative to NW1 and refer to the martensite lattice. From table 1, it is evident that NW1 and NW2 are in exact coincidence, as are NW3 and NW4.

TABLE 1

The Axis-Angle pairs relating Martensite lattices which are variants of the Nishiyama-Wasserman Orientation Relationship.

	Variant		Rotation axis			Rotation Angle
NW1	$(\bar{1}10)_\alpha \parallel (\bar{1}11)_\gamma$	$[001]_\alpha \parallel [0\bar{1}1]_\gamma$				
NW2	$(110)_\alpha \parallel (\bar{1}11)_\gamma$	$[001]_\alpha \parallel [0\bar{1}1]_\gamma$	-1.0000	0.0000	0.0000	90.00
NW3	$(110)_\alpha \parallel (1\bar{1}1)_\gamma$	$[001]_\alpha \parallel [011]_\gamma$	-0.9856	-0.1692	0.0000	90.00
NW4	$(110)_\alpha \parallel (11\bar{1})_\gamma$	$[001]_\alpha \parallel [011]_\gamma$	-0.9856	-0.1692	0.0000	90.00

For the Kurdjumov-Sachs orientation relationship, exact matching was never obtained, although some variants were closely related.

It thus seems possible to generate crystallographically indistinguishable ferrite crystals (in a given γ grain), each of whose specific lattice correspondence with respect to the austenite is different, although crystallographically equivalent. It should be emphasized that while NW1 and NW2 cannot be crystallographically differentiated, their shape strains must differ. It would therefore seem possible for these crystals to grow adjacently in a manner such that their shape strains mutually accommodate. In fact, certain thermoelastic martensites exhibit precisely this kind of behaviour; the martensite plates mutually accommodate so that long range stresses in the matrix are reduced or eliminated, thereby allowing the transformation to proceed at a relatively low driving force. This seems to be true not only when the transformation crystallography is degenerate, in the sense that opposite shape deformations may possess a common habit plane (13,14), but also when a number of variants with crystallographically equivalent but specifically different habit planes group in back-to-back self-accommodating formations (15). It is felt that the latter situation applies in the case of Widmanstätten ferrite. The formation of mutually accommodating back-to-back Widmanstätten plates would not only explain the tent-like surface relief, but also the fact that the opposite faces of Widmanstätten plates often have different crystallographic indices (see for instance, fig. 12, ref. 4). It is possible that these two faces represent the habit plane variants of the proposed back-to-back component plates. In this respect, it is interesting to note that NW1 and NW2 both have a common $(\bar{1}11)_\gamma$ plane to which their respective ferrite planes of the form $\{110\}_\alpha$ are parallel. Since the habit plane of Widmanstätten ferrite (3) lies close to the $\{\bar{1}11\}_\gamma$ which is parallel to $\{110\}_\alpha$, NW1 and NW2 can be expected to have habit plane poles which symmetrically cluster about a common $(\bar{1}11)_\gamma$ pole, as would be necessary for simultaneous back-to-back growth in a manner consistent with the observed thin wedge shape of Widmanstätten ferrite.

The above considerations seem to be able to explain the tent-like relief of Widmanstätten ferrite plates, and tend to support Watson and McDougall's (3) belief that such plates form by a displacive mechanism (although carbon diffusion would be allowed). In the light of the present results, it is pertinent to reconsider available data which are claimed to support a diffusional growth mechanism.

Aaronson et al. (16) suggest that if the shape strain of Widmanstätten ferrite is produced by a displacive mechanism, and is elastically accommodated, then the associated strain energy is too high to permit any transformation at the Widmanstätten start temperature. McDougall (17) criticized this argument on the basis that plastic relaxation must act to relieve the elastic strain energy at the temperatures where transformation occurs. The present work suggests another strain energy reduction method, i.e. by the simultaneous formation of mutually accommodating plates.

The existence of surface relief effects accompanying Widmanstätten ferrite formation is generally accepted. However, the diffusional school consistently fails to explain the mechanism of relief production. The proposition (4) that invariant plane strain (IPS) relief arises simply due to the existence of a sessile semi-coherent interface is inadequate, and also leads to the following discrepancies:

1. IPS relief is not obtained during the massive transformation in iron and its alloys, nor in non-ferrous alloys, despite the fact that a Widmanstätten ferrite type ledge mechanism is considered to be operative (18).
2. IPS relief is not obtained during the interphase precipitation reactions, where it has been convincingly demonstrated that a ledge mechanism operates (19,20).

There is a further serious inconsistency in the interpretation of shape changes. From their earlier arguments (16), the proponents of the diffusional mechanism imply that no strain energy can be associated with a shape change when the latter (somehow) arises due to a diffusional transformation. It is on this basis that they claim (16) the thermodynamic impossibility of a displacive mechanism. However, it now seems that the same strain energy term is being associated even with a "diffusionally produced shape change" (21), and on the considerations of (16), diffusional transformation would also become impossible. In fact, the confusion only arises due to the failure of the diffusional mechanism to explain the shape change and its implications.

Rigsbee and Aaronson (22) determined the interfacial structure of the Widmanstätten ferrite-austenite interfaces in an Fe-Si-C alloy. They found that the broad faces of the plates consist of arrays of parallel sessile anti-coherency dislocations (23) and parallel triatomic structural ledges. The risers of the latter features were found to be coherent, and it was suggested that these ledges are also sessile since they serve to maximize the matching across the interface. The deduced sessile nature of the α/γ interfaces led Rigsbee and Aaronson to conclude that the displacive mechanism for ferrite formation is impossible since such a mechanism requires a glissile interface. However, we note that the risers of the above ledges are regions of forced elastic coherency between the α/γ lattices. They should therefore contain coherency dislocations (23) and should in fact be glissile. Furthermore, their motion would result in displacive transformation and would explain the observed shape change associated with Widmanstätten ferrite formation. The contention (22) that such ledges must be immobile since their motion would change the boundary structure is unjustified; the movement of these uniformly spaced coherent ledges in unison would maintain the boundary structure, and at the same time accomplish displacive transformation. The driving force for such ordered motion would be the need to maintain a low interfacial energy.

Finally, we consider the criticism (16) that the observed habit plane scatter of Widmanstätten ferrite (3) is inconsistent with the phenomenological theory of displacive transformation (24,25). Since the lattice parameter of the austenite continuously changes with transformation (due to the partitioning of carbon), such scatter is only to be expected; the habit plane predicted by theory (24,25) is a function of the ratio of the γ,α lattice parameters.

$$(hkl)_{\alpha NW1} = (hkl)_\gamma \begin{pmatrix} \overline{.16910} & \overline{.98560} & 0 \\ \overline{.69692} & .11951 & \overline{.70711} \\ \overline{.69692} & .11951 & .70711 \end{pmatrix}$$

$$(hkl)_{\alpha NW2} = (hkl)_\gamma \begin{pmatrix} .16910 & \overline{.98560} & 0 \\ .69692 & .11951 & \overline{.70711} \\ .69692 & .11951 & .70711 \end{pmatrix}$$

General Summary

The present work suggests the existence of crystallographic degeneracies in the FCC-BCC transformation and it has been shown that it is possible to understand the tent-like relief associated with some Widmanstätten ferrite plates in terms of the formation of back-to-back mutually accommodating variants. It should be noted that the general arguments presented in this paper should also be applicable to the bainite and martensite transformations in low alloy steels. The crystallographic analysis and other considerations indicate that the surface relief of Widmanstätten ferrite can be understood in terms of a displacive transformation mechanism. This hypothesis has been discussed in terms of previous work.

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