LBL-11803 c.2
Preprint

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Materials & Molecular Research Division

Submitted to Scripta Metallurgica

FURTHER DISCUSSION OF ORIENTATION RELATIONSHIPS, SURFACE RELIEFS AND FCC-BCC TRANSFORMATIONS IN STEELS

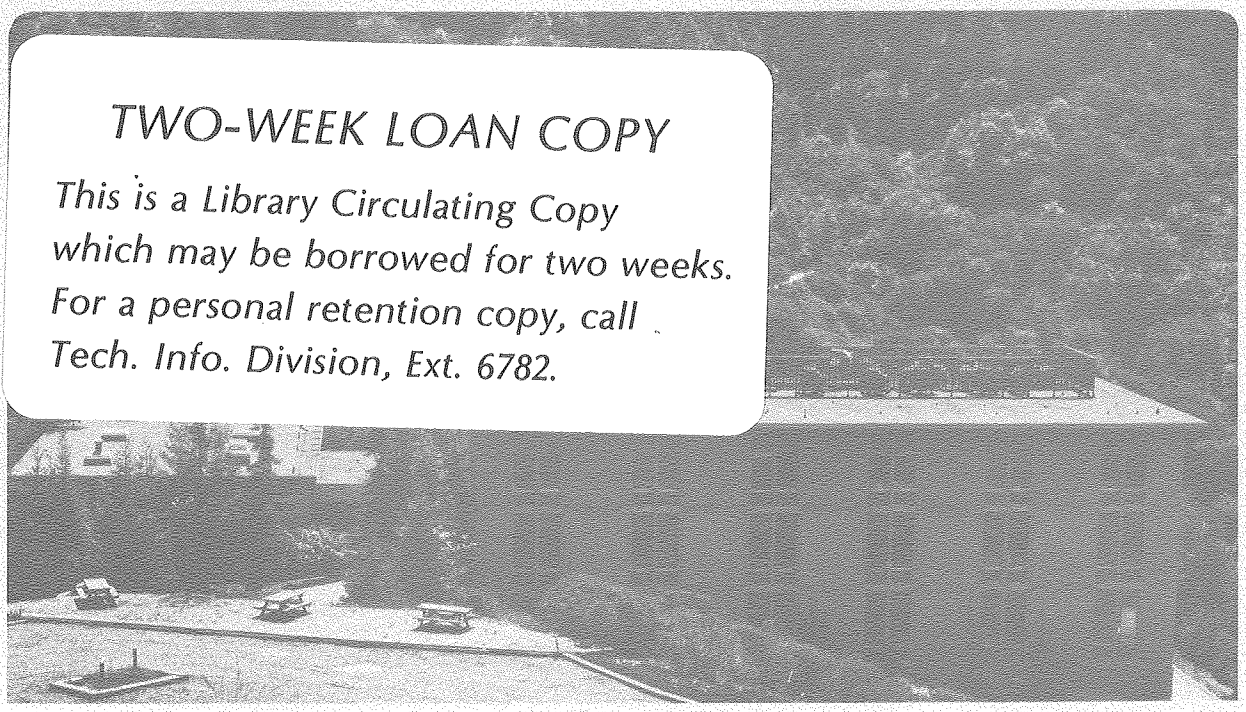
U. Dahmen

November 1980

RECEIVED
LAWRENCE
BERKELEY LABORATORY

JAN 7 1981

LIBRARY AND
DOCUMENTS SECTION



TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 6782.

LBL-11803 c.2

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

FURTHER DISCUSSION OF ORIENTATION RELATIONSHIPS, SURFACE RELIEFS AND FCC-BCC TRANSFORMATIONS IN STEELS

U. Dahmen

Materials and Molecular Research Division,
Lawrence Berkeley Laboratory,
Department of Materials Science and Mineral Engineering
University of California, Berkeley, California 94720

In a recent communication (1) Bhadeshia gives an explanation of the tent-shaped surface relief effects observed in association with Widmanstätten ferrite (2, 3) and lower bainite. Based on his proposed explanation he concludes that the diffusional fcc → bcc transformation in steel takes place by a displacive mechanism. This conclusion is disputed by Aaronson (4) in a letter following that of Bhadeshia by showing that the experimentally observed orientation relationships are different from the one (Nishyama-Wassermann (N-W), necessary for Bhadeshia's mechanism. He therefore holds that the transformation is purely diffusional and that "any attempts to understand diffusional phase transformations in terms of a shear mechanism are counterproductive."

The purpose of the present note is (1) to show that Bhadeshia's mechanism seems to be based on a misinterpretation of the lattice symmetries resulting from the fcc → bcc transformation and cannot explain a tent-shaped surface relief even if the N-W orientation relationship is followed, and (2) to suggest that attempts to formally understand diffusional phase transformations in terms of shear may not always be counterproductive.

The conditions for crystallographic degeneracy

The mechanism Bhadeshia proposes is based on the idea of crystallographic degeneracy which exists for fcc → hcp martensitic transformations:

the same crystal orientation of the hcp phase can be produced from a fixed fcc parent lattice in three distinct ways. This is shown in a two-dimensional sketch in Fig. 1. The triangles represent a {111} plane in the fcc parent lattice, the hexagons are the basal planes of the hcp product and the arrows indicate the Burgers vectors of the Shockley partials which shear the fcc into an hcp lattice. Crystallographically, the three configurations shown in Figs. 1a, b, and c are identical because they are related by symmetry operations of both the matrix and the product, namely a 120° rotation. Macroscopically, however, the three cases would give quite different results. The simple shear described by the direction of the Shockley partials does not share the threefold symmetry common to the matrix and the product. The macroscopic shape change in the direction of the arrows, which accompanies the transformation will therefore be different for a, b, and c. This is the degeneracy described by Bhadeshia.

He shows that a combination of these three degenerate transformations allows for an overall accommodation of the macroscopic transformation strain. However, he then suggests that a similar degeneracy exists for the fcc $\rightarrow$ bcc transformation. Using the N-W orientation relationship (shown in Fig. 2), he calculates misorientations between all 24 variants, searching for degenerate pairs, i.e. ferrite crystals in identical orientation but produced by different transformation strains. He finds two such degenerate pairs of variants which he calls NW1/NW2 and NW3/NW4. He suggests that these are responsible for the observed surface relief and that therefore the transformation must be displacive in nature.

While the principle of his explanation is attractive, the specific mechanism does not seem possible. One pair of variants, NW3/NW4, is not

degenerate since it consists of ferrite crystals in different orientations. This is obvious from the fact that NW3 and NW4 have (110) planes parallel to two different {111} planes of the parent and thus make an angle of 70.5° instead of 60°. The other pair, NW1/NW2, is crystallographically identical, but does not have the necessary difference in the shape deformations. This is illustrated in Fig. 3 which represents two-dimensional projections of the N-W orientation relationship viewed along the three orthogonal coincident poles shown in the stereogram in Fig. 2. For each of these poles, the symmetries of the fcc parent, the bcc product, and the strain are indicated separately by the appropriate symbols. The two variants called NW1 and NW2 are crystallographically identical; they are related by a 90° rotation around $[001]$ bcc (see Fig. 3b). By careful inspection of the stereogram (Fig. 2), it can be seen that this 90° rotation of the product alone is equivalent to a 180° rotation of parent and product together around the third coincident pole ($[\bar{1}10]$ bcc $[\bar{1}2\bar{1}]$ fcc). The latter rotation is the symmetry operation of the parent which produces NW2 from NW1. From Fig. 3c it can be seen that around this axis, the product and the strain have the same two-fold rotational symmetry. Hence the shape deformation will be identical for NW1 and NW2 and their degeneracy cannot account for any surface relief.

This failure of an analogy with the degeneracy fcc $\rightarrow$ hcp transformations can be understood in more general terms when analysed in the context of Cahn's (5) treatment of the symmetry of martensites. He distinguishes between the symmetries of the parent, the product and the strain and shows that the crystallographic symmetry of a transformation product is usually a subgroup of (i.e. lower than) both the symmetry of the parent <u>and</u> that of the strain. Only for specific values of the strain

is it possible to form a supergroup (i.e. higher or equal symmetry). This is the case for both types of transformation considered here as seen in Fig. 1 where a three-fold axis in the parent becomes sixfold in the product, or in Fig. 3b where a twofold axis becomes fourfold. Thus both transformations lead to special configurations for which along certain axes the parent and the product have common symmetry operation. Fig. 1 and Figs. 3b and c show projections along these axes. However, in Fig. 3, the symmetry common to the two crystal lattices is also shared by the strain and hence by the shape deformation. Therefore these two crystallographically degenerate variants cannot have different shape strains and are unable to explain a tent-shaped surface relief effect. From Fig. 1 it is clear why this is different for the fcc → hcp transformation. Here the symmetry of the strain is lower than the threefold axis common to parent and product lattices. It is now possible to state a general condition for the occurrence of a crystallographic degeneracy allowing an overall accommodation of the shape change - there must be at least one symmetry element common to parent and product (matrix and precipitate) which is not shared by the transformation strain.

This is a rare occurrence since usually the symmetry of the product is lower than those of both parent and strain (5). Plotting symmetry diagrams for the principal axes of a transformation as illustrated in Fig. 3, shows that even the fcc → bcc transformation of the highest symmetry, the one describing the Bain orientation relationship, does not fulfill the given condition. The same is true for the low-symmetry K-S orientation relationship.

Diffusional transformations and shear

The symmetry arguments presented above agree with Aaronson's response since they give one more reason why Bhadeshia's conclusion of a shear mechanism for the transformation seems unfounded. His conclusion is different, however, from the use of lattice shear as a purely formal aid in the understanding of the crystallography and morphology of precipitation. Martensite (6) and O-lattice (7) theories are both basically geometrical. Formally applied to diffusion controlled transformations, both theories have been very successful at times. In fact, Aaronson and co-workers have achieved remarkable agreement with experimentally observed interface structures and morphologies in diffusion controlled transformations using O-lattice theory (8) as well as graphical (9) and computerized (10) models similar to O-lattice theory. The fact that the matrix algebra description of the total transformation may involve a shear does not necessarily mean that the transformation actually proceeds by a shear mechanism. For example, mathematically, the transformation matrix relating the parent to the product may look identical for a martensitic and a diffusion controlled transformation while the mechanism of transformation is fundamentally different. Traditionally, a successful analysis of a phase transformation by martensite theory has always involved the conclusion that the structural change proceeds martensitically. The paper by Bhadeshia (1) discussed above, Wayman and Van Landuyt's analysis of oxide plates in Ta (11), or Watson and McDougall's (2) study of Widmanstätten ferrite are typical examples of this tradition. In this sense, Hoekstra's (12) recent demonstration of the failure of martensite theories in explaining the crystallography of bainite plates defeats only the notion that the bainite reaction proceeds by a martensitic shear mechanism.

It does not preclude the use of basically geometrical methods which may involve a theoretical lattice shear in the analysis of this diffusion-controlled reaction. A formal theoretical treatment of phase transformations in this manner has proved to be successful and will be published elsewhere.

Summary

In response to a recent discussion in this journal concerning tent-shaped surface-relief effects and the mechanism of formation of Widmanstätten ferrite and lower bainite, it was shown that Bhadeshia's (1) explanation of surface reliefs is in error. A degeneracy of the fcc → hcp type does not exist for an fcc → bcc transformation. Based on a distinction between the symmetries of the matrix, the transformation product and the strain (5), a general rule was derived for the occurrence of the type of crystallographic degeneracies described by Bhadeshia. The present analysis confirmed Aaronson's (4) contention that the transformation is not shear-like (martensitic) in nature but diffusion controlled. It was argued, however, that the formal treatment of diffusional transformations may involve a shear.

Acknowledgements

I would like to thank Dr. Ken Westmacott for his interest and support and for critically reviewing the manuscript. Thanks are also due to Dr. Lee Tanner and Alan Pelton for helpful discussions. The work was supported by the Division of Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy under Contract Number W-7405-Eng-48.

References

1. H. K. D. H. Bhadeshia, Scripta Met. 14, 821 (1980).

2. J. D. Watson and P. G. McDougall, Acta Met. 21, 961 (1973).

3. K. R. Kinsman, E. Eichen, and H. I. Aaronson, Met. Trans. 6A, 303 (1975).

4. H. I. Aaronson, Scripta Met. 14, 825 (1980).

5. J. W. Cahn, Acta Met. 25, 721 (1977).

6. J. S. Bowles, and J. K. Mackenzie, Acta Met. 2, 129 (1954).

7. W. Bollmann, Crystal Defects and Crystalline Interfaces, Springer, N. Y. (1970).

8. M. R. Plichta and H. I. Aaronson, Acta Met. 28, 1041 (1980).

9. M. G. Hall, H. I. Aaronson and K. R. Kinsman, Surf. Sci. 31, 257 (1972).

10. J. M. Rigsbee and H. I. Aaronson, Acta Met. 27, 351 (1979).

11. C. M. Wayman and J. Van Landuyt, Acta Met. 16, 815 (1968).

12. S. Hoekstra, Acta Met. 28, 507 (1980).

Figure Captions

Fig. 1. Three different ways of producing the same hcp lattice from an fcc crystal by three different simple shears, indicated by arrows. The three configurations in a, b, and c are related by 120° rotations which leave the parent and the product unchanged but lead to distinct (shape) strains.

Fig. 2. Nishiyama-Wassermann (N-W) orientation relationship showing a superposition of a (111) fcc projection (solid circles) and a (110) bcc projection (open circles). The three coincident poles define the orientation relationship. The fcc poles are underlined.

Fig. 3. Symmetry diagram of the three coincident poles of the N-W orientation relationship shown in Fig. 2. The (shape) strain has orthorhombic symmetry and hence three orthogonal axes with twofold symmetry. In contrast to Fig. 1, a rotation of 180° around the symmetry axes b, and c will leave parent, product and (shape) strain unchanged.

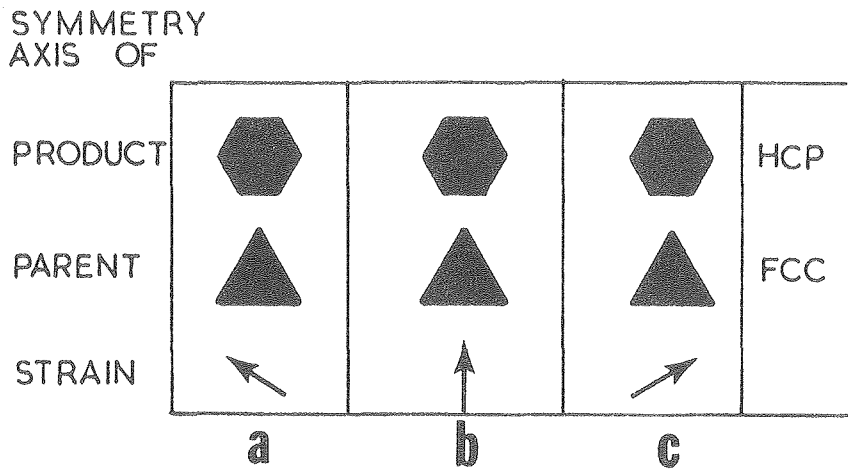

SYMMETRY
AXIS OF
PRODUCT
PARENT
STRAIN
HCP
FCC
a
b
c

Fig. 1

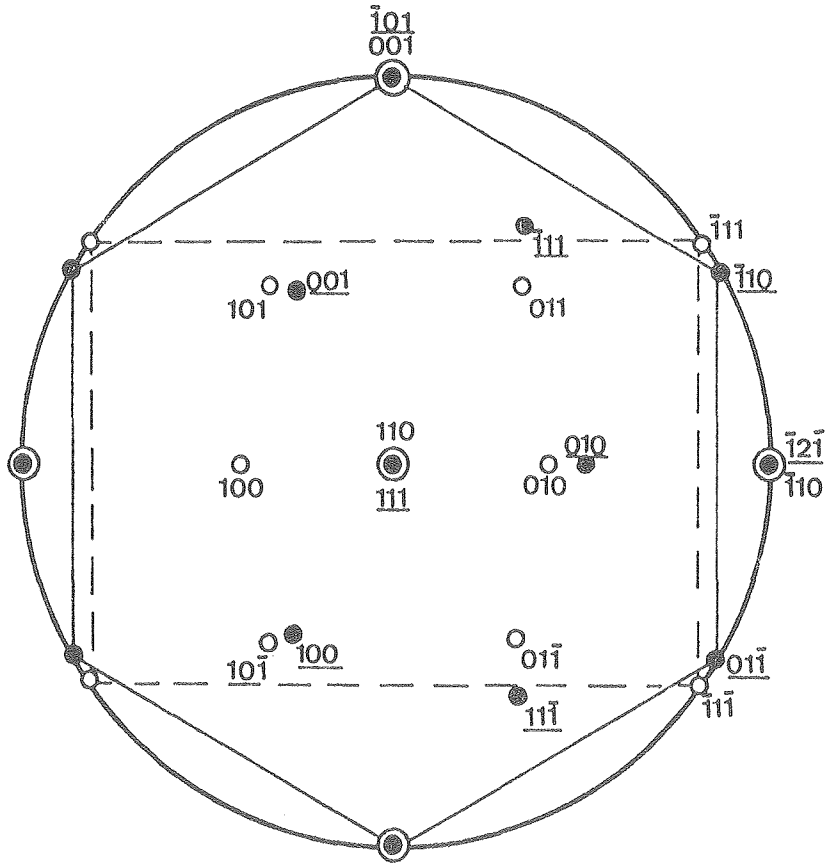

$\bar{1}01$
001
$\bar{1}11$
$\bar{1}11$
$\bar{1}10$
101
001
011
110
100
111
010
010
$\bar{1}2\bar{1}$
$\bar{1}10$
$10\bar{1}$
100
$01\bar{1}$
$01\bar{1}$
$11\bar{1}$
$\bar{1}1\bar{1}$

Fig. 2

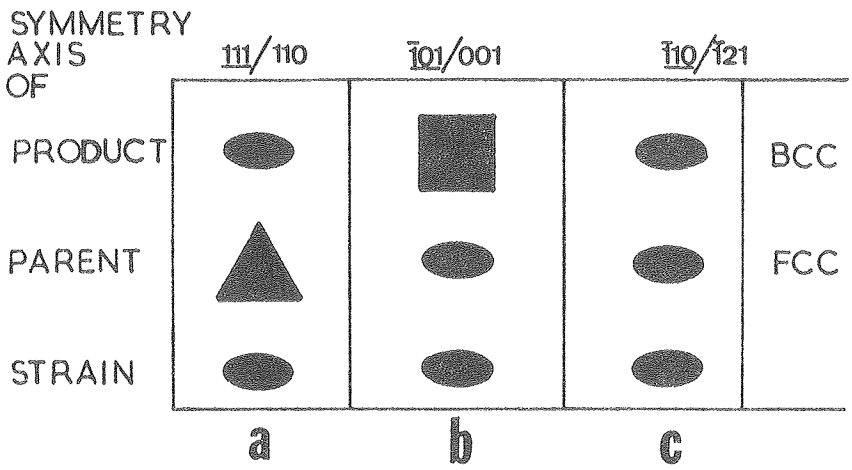

SYMMETRY
AXIS
OF
111/110
$\bar{1}01$/001
$\bar{1}10$/$\bar{1}21$
PRODUCT
PARENT
STRAIN
BCC
FCC
a
b
c

Fig. 3